



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2025 – 02:46 PM JST

PDB ID : 9JZF / pdb_00009jzf
Title : Crystal structure of OsSPS3 complexed with zoledronate and isopentenyl diphosphate
Authors : Xiao, H.; Li, M.; Yang, G.-F.
Deposited on : 2024-10-14
Resolution : 2.45 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

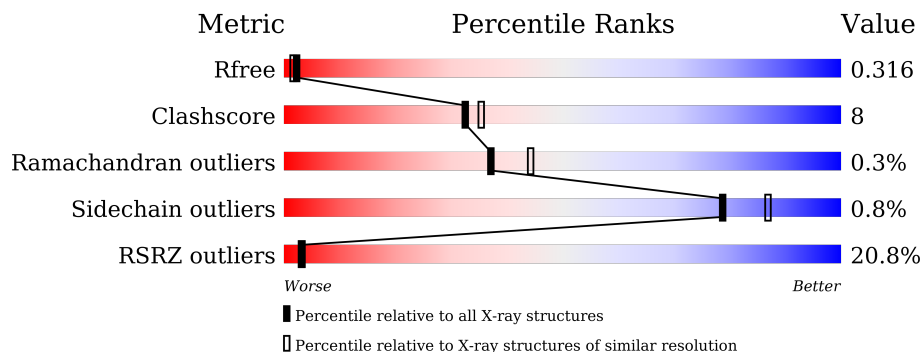
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	324	<div> <div>10%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
1	B	324	<div> <div>28%</div> <div> <div></div> <div>71%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

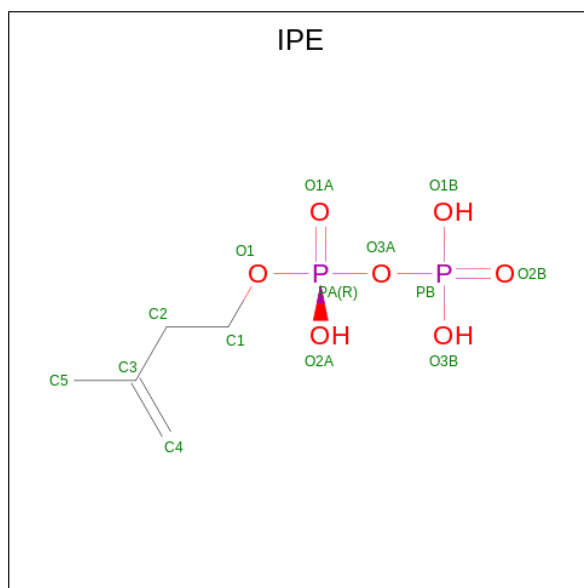
There are 5 unique types of molecules in this entry. The entry contains 4660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable solanesyl-diphosphate synthase 3, chloroplastic.

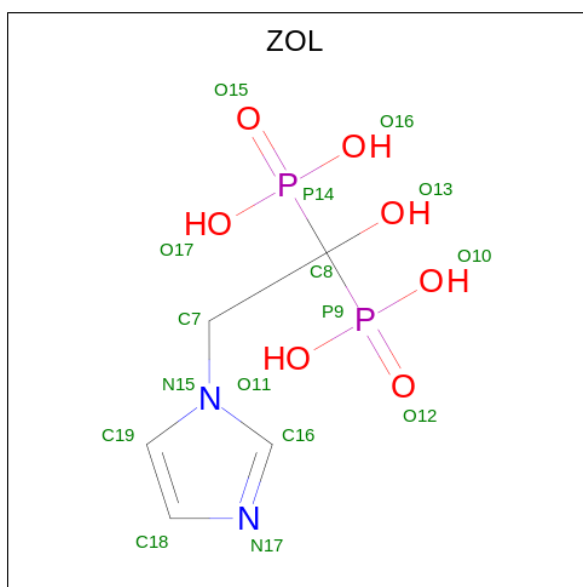
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2489	1571	421	489	8			
1	B	283	Total	C	N	O	S	0	0	0
			2115	1334	356	417	8			

- Molecule 2 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (CCD ID: IPE) (formula: $C_5H_{12}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 3 is ZOLEDRONIC ACID (CCD ID: ZOL) (formula: $C_5H_{10}N_2O_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	5	2	7	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		

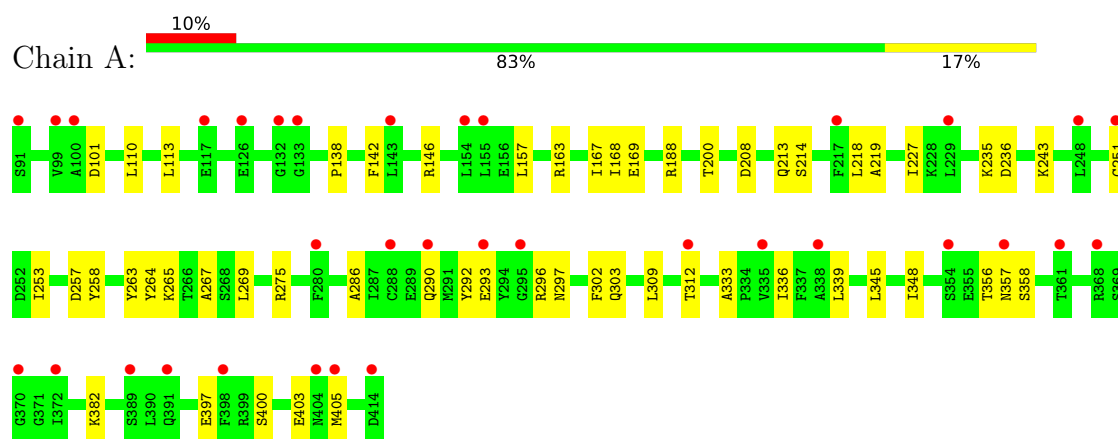
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	5	Total	O	0	0
			5	5		

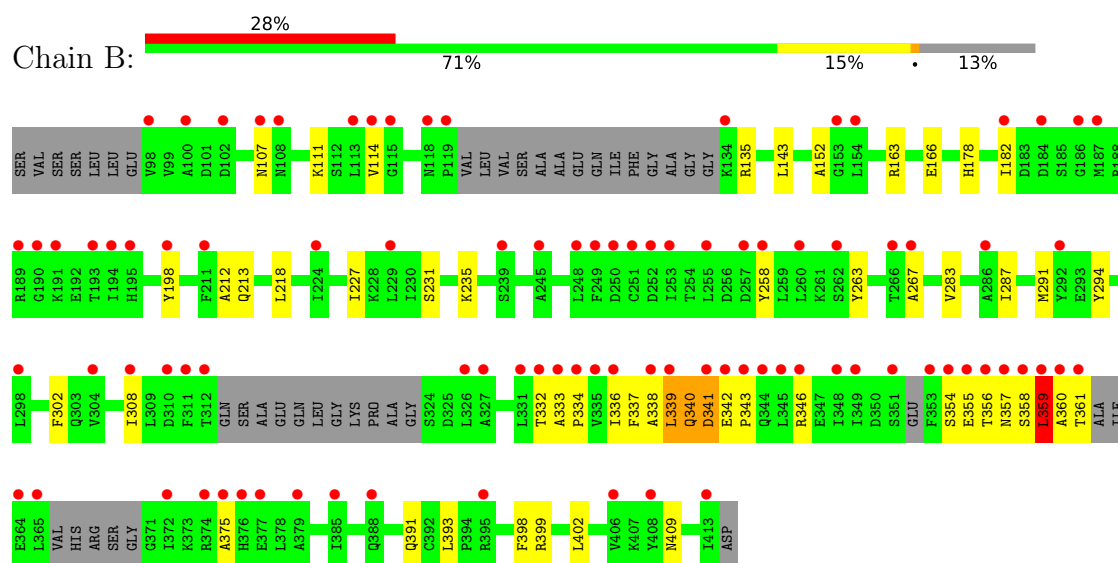
3 Residue-property plots [i](#)

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: Probable solanesyl-diphosphate synthase 3, chloroplastic



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.05Å 90.72Å 125.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.45 48.29 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.29-2.45) 98.7 (48.29-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.261 , 0.318 0.262 , 0.316	Depositor DCC
R_{free} test set	1225 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4660	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: IPE, MG, ZOL

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	0.10	0/2522	0.29	0/3410
1	B	0.36	0/2138	0.66	4/2894 (0.1%)
All	All	0.25	0/4660	0.49	4/6304 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	LEU	N-CA-C	-7.71	103.97	113.15
1	B	340	GLN	N-CA-C	-6.53	101.62	111.34
1	B	337	PHE	N-CA-C	-6.41	104.72	112.54
1	B	346	ARG	N-CA-C	-5.27	104.96	111.33

There are no chirality outliers.

There are no planarity outliers.

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	2489	0	2502	40	0
1	B	2115	0	2046	37	0
2	A	14	0	9	3	0
3	A	16	0	6	1	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	18	0	0	0	0
5	B	5	0	0	1	0
All	All	4660	0	4563	72	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 (72) 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:B:355:GLU:C	1:B:357:ASN:H	1.92	0.76
1:B:355:GLU:O	1:B:357:ASN:N	2.22	0.72
1:A:356:THR:O	1:A:357:ASN:ND2	2.23	0.72
1:A:309:LEU:HA	1:A:312:THR:HG22	1.73	0.70
1:B:263:TYR:HA	1:B:267:ALA:HB3	1.72	0.70
1:A:218:LEU:HD21	1:A:227:ILE:HA	1.74	0.70
1:A:138:PRO:HG3	1:A:169:GLU:HB2	1.73	0.69
1:A:263:TYR:HA	1:A:267:ALA:HB3	1.76	0.68
1:A:146:ARG:HG2	1:A:157:LEU:HD11	1.76	0.67
1:B:393:LEU:HB2	1:B:399:ARG:HG3	1.78	0.65
1:B:338:ALA:C	1:B:340:GLN:H	2.05	0.64
1:B:355:GLU:C	1:B:357:ASN:N	2.56	0.64
1:B:341:ASP:O	1:B:342:GLU:C	2.39	0.63
1:B:338:ALA:O	1:B:340:GLN:N	2.32	0.62
1:A:348:ILE:HG23	1:A:358:SER:HB2	1.82	0.62
1:B:333:ALA:HA	1:B:336:ILE:HG22	1.81	0.62
1:B:218:LEU:HG	1:B:227:ILE:HG12	1.83	0.59
1:A:293:GLU:OE2	1:A:296:ARG:NH2	2.36	0.58
1:B:111:LYS:HA	1:B:114:VAL:HG12	1.85	0.58
1:B:338:ALA:C	1:B:340:GLN:N	2.59	0.58
1:A:251:CYS:HB3	1:A:339:LEU:HD21	1.86	0.56
1:B:143:LEU:HD23	1:B:398:PHE:HD2	1.72	0.54
1:B:152:ALA:HB2	1:B:283:VAL:HG12	1.90	0.52
1:B:357:ASN:C	1:B:359:LEU:H	2.15	0.52
1:B:182:ILE:HG13	1:B:198:TYR:HD1	1.75	0.51
1:A:208:ASP:OD2	1:B:178:HIS:ND1	2.29	0.51
1:A:219:ALA:HA	1:A:227:ILE:HD11	1.93	0.50
1:B:107:ASN:ND2	5:B:502:HOH:O	2.44	0.49
1:A:167:ILE:HG23	1:A:214:SER:HB3	1.94	0.49
1:A:243:LYS:NZ	1:A:257:ASP:O	2.45	0.49
1:A:275:ARG:HB2	1:A:292:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASN:C	1:B:359:LEU:N	2.72	0.48
1:A:286:ALA:O	1:A:290:GLN:HG2	2.13	0.48
1:B:332:THR:OG1	1:B:334:PRO:HD2	2.14	0.48
1:B:341:ASP:O	1:B:343:PRO:N	2.46	0.48
1:A:235:LYS:NZ	1:B:213:GLN:OE1	2.33	0.47
1:B:354:SER:OG	1:B:355:GLU:N	2.47	0.47
1:A:218:LEU:CD2	1:A:227:ILE:HA	2.44	0.47
1:A:200:THR:OG1	1:B:182:ILE:O	2.33	0.47
1:A:339:LEU:HD12	1:A:345:LEU:HB3	1.95	0.47
1:A:236:ASP:O	1:A:264:TYR:HB3	2.15	0.46
1:A:397:GLU:HA	1:A:400:SER:OG	2.15	0.46
1:A:101:ASP:OD2	1:A:101:ASP:N	2.47	0.46
1:B:227:ILE:O	1:B:231:SER:OG	2.30	0.46
1:A:400:SER:HA	1:A:403:GLU:HB2	1.98	0.46
1:A:163:ARG:O	1:A:167:ILE:HG13	2.15	0.46
1:A:303:GLN:HE22	2:A:501:IPE:H51	1.81	0.45
1:A:168:ILE:HG23	1:A:269:LEU:HD11	1.99	0.45
1:A:297:ASN:HB3	1:A:382:LYS:O	2.17	0.45
1:B:163:ARG:HA	1:B:166:GLU:HG2	2.00	0.44
1:A:303:GLN:NE2	2:A:501:IPE:H51	2.31	0.44
1:A:110:LEU:HD23	1:A:113:LEU:HD22	2.00	0.43
1:A:405:MET:HE2	1:A:405:MET:HB3	1.78	0.43
1:A:253:ILE:HG23	1:A:336:ILE:HD11	1.98	0.43
1:B:258:TYR:CE2	1:B:333:ALA:HB2	2.53	0.43
1:B:358:SER:C	1:B:360:ALA:H	2.26	0.43
1:A:235:LYS:HA	1:B:212:ALA:HB1	2.00	0.43
1:B:287:ILE:O	1:B:291:MET:HG2	2.18	0.43
1:B:391:GLN:OE1	1:B:399:ARG:NH1	2.52	0.43
1:A:113:LEU:HD12	1:A:113:LEU:HA	1.90	0.43
1:A:302:PHE:HE1	2:A:501:IPE:H53	1.83	0.42
1:B:359:LEU:HD13	1:B:359:LEU:HA	1.83	0.42
1:A:188:ARG:NH1	3:A:502:ZOL:O16	2.37	0.41
1:A:258:TYR:CE2	1:A:333:ALA:HB2	2.55	0.41
1:B:308:ILE:HD11	1:B:375:ALA:HB1	2.01	0.41
1:A:382:LYS:HD3	1:A:382:LYS:HA	1.82	0.41
1:A:142:PHE:O	1:A:146:ARG:HG3	2.21	0.41
1:A:213:GLN:OE1	1:B:235:LYS:HD2	2.20	0.41
1:B:302:PHE:HA	1:B:409:ASN:HD21	1.85	0.41
1:A:265:LYS:NZ	1:A:303:GLN:OE1	2.51	0.40
1:B:294:TYR:CE2	1:B:402:LEU:HD22	2.56	0.40
1:B:135:ARG:HD3	1:B:135:ARG:H	1.86	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	322/324 (99%)	311 (97%)	11 (3%)	0	100	100
1	B	271/324 (84%)	254 (94%)	15 (6%)	2 (1%)	19	22
All	All	593/648 (92%)	565 (95%)	26 (4%)	2 (0%)	37	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	LEU
1	B	356	THR

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	269/272 (99%)	269 (100%)	0	100	100
1	B	218/272 (80%)	214 (98%)	4 (2%)	54	67
All	All	487/544 (90%)	483 (99%)	4 (1%)	79	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	339	LEU

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Mol	Chain	Res	Type
1	B	341	ASP
1	B	359	LEU
1	B	361	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	B	118	ASN
1	B	388	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	IPE	A	501	-	11,13,13	2.32	1 (9%)	15,19,19	1.87	3 (20%)
3	ZOL	A	502	4	14,16,16	2.41	6 (42%)	20,26,26	1.82	6 (30%)

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	IPE	A	501	-	-	7/13/13/13	-
3	ZOL	A	502	4	-	1/23/23/23	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IPE	C4-C3	7.06	1.53	1.33
3	A	502	ZOL	P14-O16	-4.45	1.46	1.54
3	A	502	ZOL	O13-C8	-3.80	1.39	1.44
3	A	502	ZOL	C19-N15	-3.41	1.31	1.37
3	A	502	ZOL	P14-O17	-3.12	1.49	1.54
3	A	502	ZOL	P9-O10	-2.83	1.49	1.54
3	A	502	ZOL	P9-O11	-2.79	1.49	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IPE	C5-C3-C4	-4.81	111.38	121.98
3	A	502	ZOL	O11-P9-C8	3.95	115.03	106.17
2	A	501	IPE	C2-C3-C4	-3.94	111.28	122.80
3	A	502	ZOL	P9-C8-P14	-3.74	106.11	112.81
2	A	501	IPE	PA-O3A-PB	-2.79	123.26	132.83
3	A	502	ZOL	O16-P14-O15	-2.65	107.11	113.06
3	A	502	ZOL	O10-P9-O12	-2.65	107.11	113.06
3	A	502	ZOL	O11-P9-O12	-2.52	107.39	113.06
3	A	502	ZOL	O17-P14-C8	2.49	111.74	106.17

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	IPE	C1-O1-PA-O2A
2	A	501	IPE	C1-O1-PA-O3A
2	A	501	IPE	C1-C2-C3-C4
2	A	501	IPE	O1-C1-C2-C3
2	A	501	IPE	C1-C2-C3-C5
2	A	501	IPE	C1-O1-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	502	ZOL	C8-C7-N15-C19
2	A	501	IPE	C2-C1-O1-PA

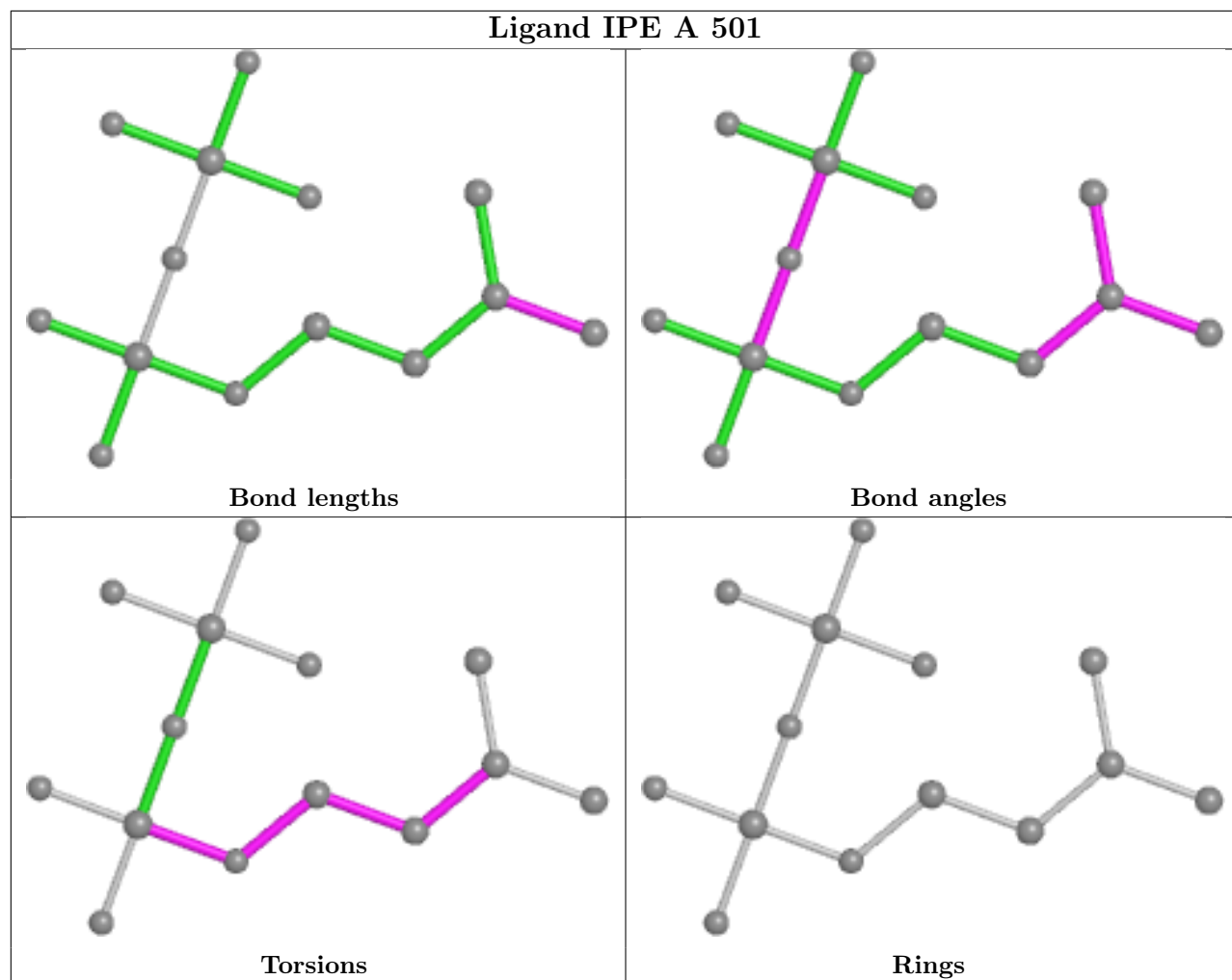
There are no ring outliers.

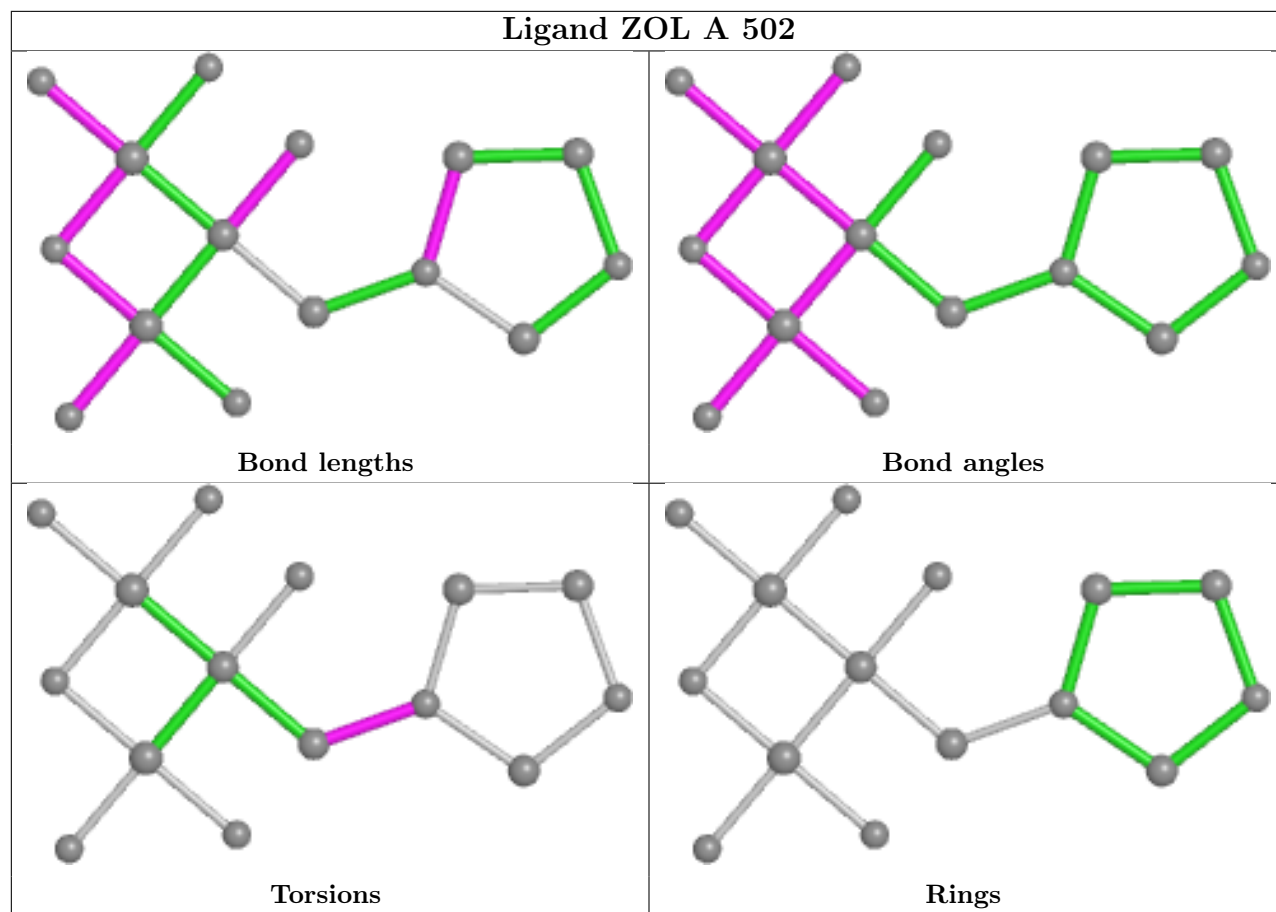
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IPE	3	0
3	A	502	ZOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IPE A 501





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	324/324 (100%)	1.06	34 (10%)	13 12	39, 55, 73, 82	0
1	B	283/324 (87%)	1.61	92 (32%)	1 1	42, 67, 98, 113	0
All	All	607/648 (93%)	1.31	126 (20%)	3 3	39, 60, 93, 113	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	TYR	4.6
1	B	311	PHE	4.6
1	B	349	ILE	4.4
1	B	339	LEU	4.2
1	B	359	LEU	4.2
1	B	335	VAL	4.2
1	B	351	SER	4.0
1	B	358	SER	3.9
1	B	334	PRO	3.8
1	B	353	PHE	3.7
1	B	356	THR	3.7
1	B	348	ILE	3.7
1	B	360	ALA	3.7
1	B	189	ARG	3.6
1	B	413	ILE	3.6
1	A	414	ASP	3.6
1	B	310	ASP	3.6
1	A	132	GLY	3.5
1	B	114	VAL	3.5
1	B	343	PRO	3.4
1	B	408	TYR	3.4
1	B	376	HIS	3.3
1	B	251	CYS	3.3
1	B	102	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	98	VAL	3.2
1	B	375	ALA	3.2
1	B	333	ALA	3.2
1	B	342	GLU	3.2
1	B	331	LEU	3.1
1	A	295	GLY	3.1
1	B	361	THR	3.1
1	B	119	PRO	3.1
1	B	336	ILE	3.1
1	B	304	VAL	3.0
1	A	398	PHE	3.0
1	B	372	ILE	3.0
1	B	134	LYS	3.0
1	B	252	ASP	2.9
1	A	312	THR	2.9
1	A	405	MET	2.9
1	B	190	GLY	2.8
1	A	338	ALA	2.8
1	B	115	GLY	2.8
1	B	260	LEU	2.8
1	B	341	ASP	2.7
1	B	365	LEU	2.7
1	B	253	ILE	2.7
1	A	117	GLU	2.7
1	A	370	GLY	2.7
1	B	258	TYR	2.7
1	B	364	GLU	2.7
1	B	292	TYR	2.7
1	B	107	ASN	2.7
1	B	262	SER	2.7
1	B	326	LEU	2.6
1	B	338	ALA	2.6
1	B	229	LEU	2.6
1	B	193	THR	2.6
1	B	344	GLN	2.6
1	B	395	ARG	2.6
1	A	357	ASN	2.6
1	B	184	ASP	2.5
1	B	388	GLN	2.5
1	A	361	THR	2.5
1	B	345	LEU	2.4
1	B	245	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	2.4
1	A	290	GLN	2.4
1	B	249	PHE	2.4
1	A	372	ILE	2.4
1	B	266	THR	2.4
1	B	312	THR	2.4
1	B	332	THR	2.4
1	B	118	ASN	2.3
1	B	357	ASN	2.3
1	A	100	ALA	2.3
1	B	255	LEU	2.3
1	B	182	ILE	2.3
1	B	195	HIS	2.3
1	B	250	ASP	2.3
1	A	288	CYS	2.3
1	A	133	GLY	2.3
1	A	154	LEU	2.3
1	B	153	GLY	2.3
1	A	293	GLU	2.3
1	B	113	LEU	2.2
1	B	248	LEU	2.2
1	B	187	MET	2.2
1	B	108	ASN	2.2
1	B	355	GLU	2.2
1	B	385	ILE	2.2
1	B	379	ALA	2.2
1	A	251	CYS	2.2
1	A	368	ARG	2.2
1	A	229	LEU	2.2
1	B	186	GLY	2.2
1	B	406	VAL	2.2
1	B	191	LYS	2.2
1	B	286	ALA	2.2
1	B	298	LEU	2.2
1	B	346	ARG	2.2
1	A	335	VAL	2.2
1	B	154	LEU	2.1
1	A	391	GLN	2.1
1	B	374	ARG	2.1
1	A	91	SER	2.1
1	B	100	ALA	2.1
1	A	217	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	126	GLU	2.1
1	B	308	ILE	2.1
1	A	143	LEU	2.1
1	A	155	LEU	2.1
1	B	211	PHE	2.1
1	B	377	GLU	2.1
1	A	389	SER	2.1
1	B	257	ASP	2.1
1	B	267	ALA	2.0
1	B	354	SER	2.0
1	B	194	ILE	2.0
1	B	224	ILE	2.0
1	A	404	ASN	2.0
1	A	248	LEU	2.0
1	A	99	VAL	2.0
1	A	280	PHE	2.0
1	A	354	SER	2.0
1	B	239	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

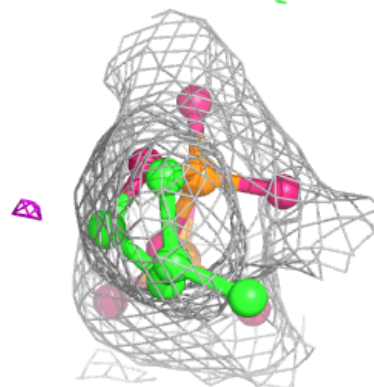
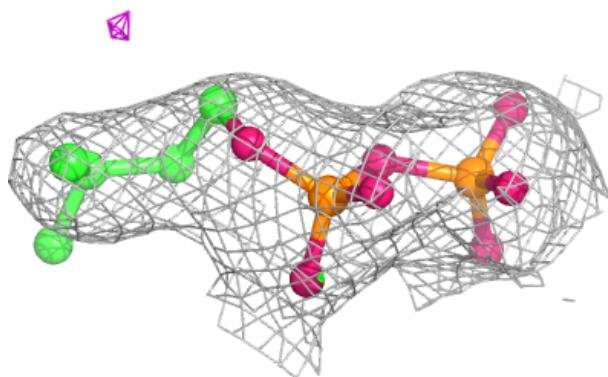
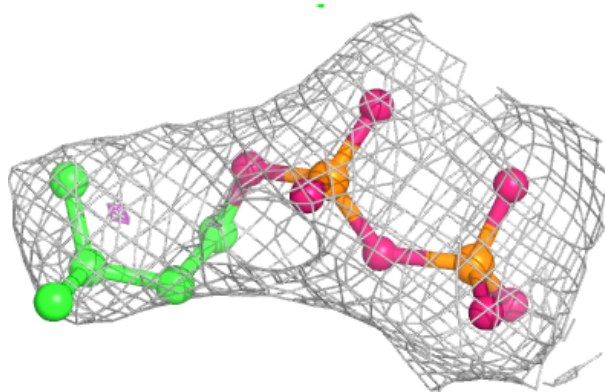
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IPE	A	501	14/14	0.91	0.13	41,52,55,62	0
3	ZOL	A	502	16/16	0.93	0.10	32,41,49,50	0
4	MG	A	504	1/1	0.93	0.07	37,37,37,37	0
4	MG	A	505	1/1	0.93	0.06	38,38,38,38	0
4	MG	A	503	1/1	0.95	0.05	41,41,41,41	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.

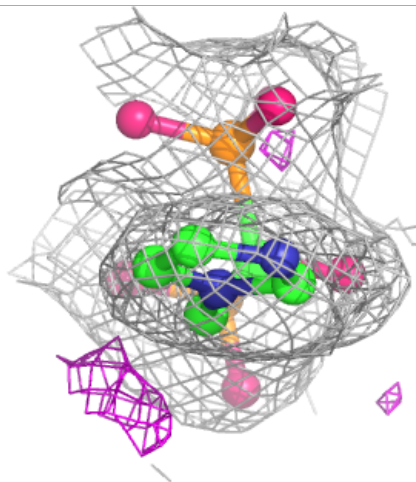
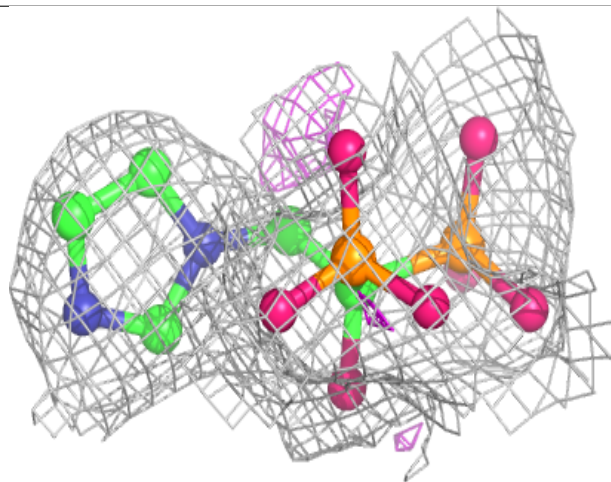
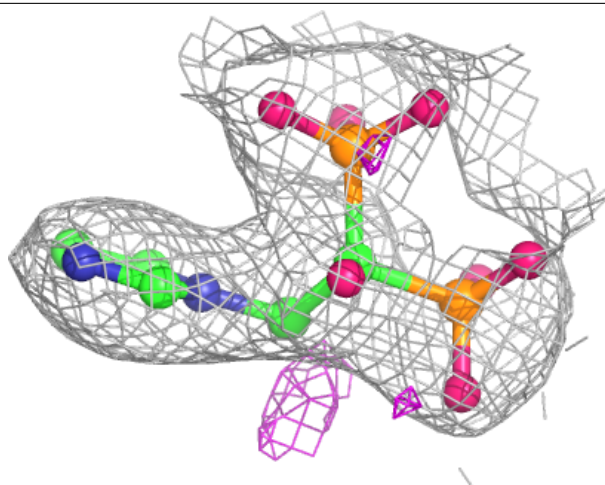
Electron density around IPE A 501:

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



Electron density around ZOL A 502:

$2mF_o-DF_c$ (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.