



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 06:15 AM EDT

PDB ID : 7A17
Title : Crystal structure of the 5-phosphatase domain of Synaptojanin1 bound to its substrate diC8-PI(3,4,5)P3 in complex with a nanobody
Authors : Paesmans, J.; Galicia, C.; Martin, E.; Versees, W.
Deposited on : 2020-08-12
Resolution : 2.73 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)
Xtrriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

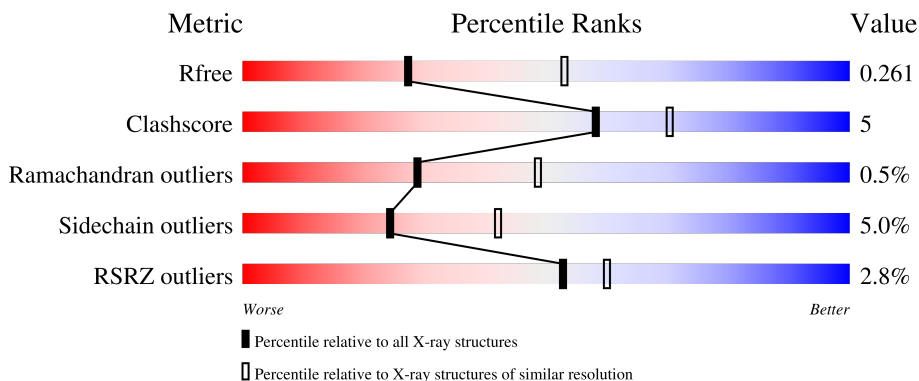
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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.



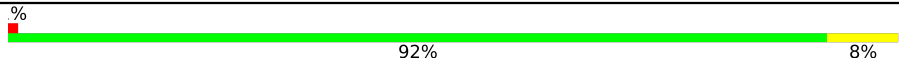
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	346	
2	B	119	
3	C	345	
3	E	345	
4	D	123	

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Mol	Chain	Length	Quality of chain
5	F	125	 <p>A horizontal bar chart representing the quality of the chain. The bar is 92% green and 8% yellow. A small red square is at the beginning of the bar. The percentage '92%' is centered below the green portion, and '8%' is centered below the yellow portion. A '%' symbol is located at the top left of the bar.</p>

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 10780 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 Isoform 2 of Synaptojanin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2708	1735	471	491	11	0	1	0

- Molecule 2 is a protein called Nanobody 13015.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	119	896	553	164	175	4	0	0	0

- Molecule 3 is a protein called Isoform 2 of Synaptojanin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	319	2581	1653	446	472	10	0	0	0
3	E	313	2537	1628	442	456	11	0	0	0

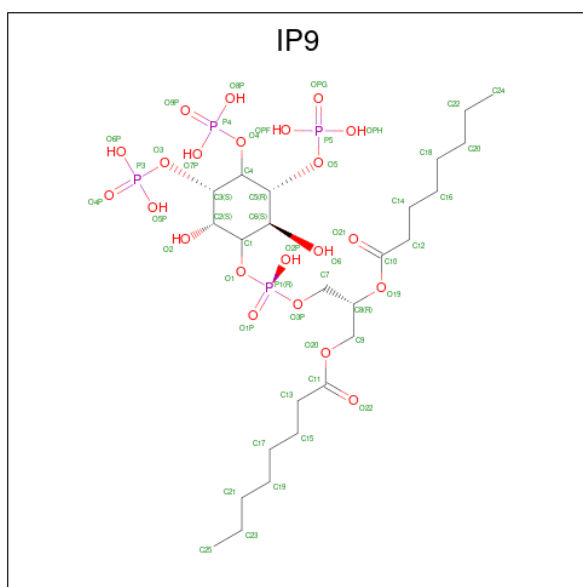
- Molecule 4 is a protein called Nanobody 13015.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	123	942	582	173	183	4	0	0	0

- Molecule 5 is a protein called Nanobody 13015.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	125	960	592	177	187	4	0	0	0

- Molecule 6 is (2R)-3-{{(R)-{{(1S,2S,3R,4S,5S,6S)-2,6-dihydroxy-3,4,5-tris(phosphonoxy)cyclohexyl}oxy}}(hydroxy)phosphoryl}oxy}propane -1,2-diyl dioctanoate (three-letter code: IP9) (formula: C₂₅H₅₀O₂₂P₄) (labeled as "Ligand of Interest" by depositor).

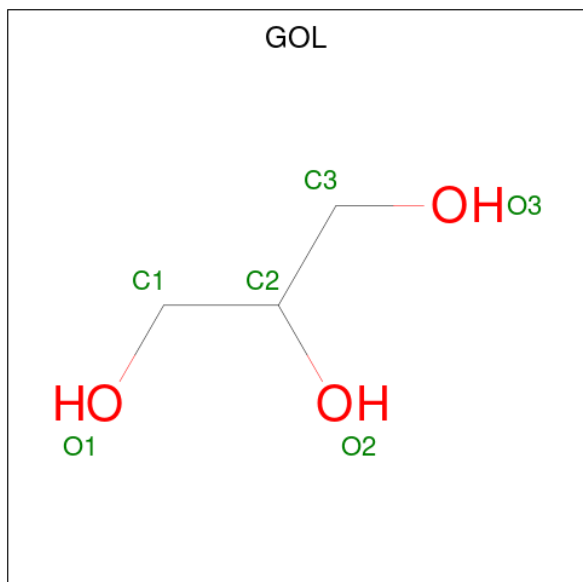


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
6	A	1	51	25	22	4	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

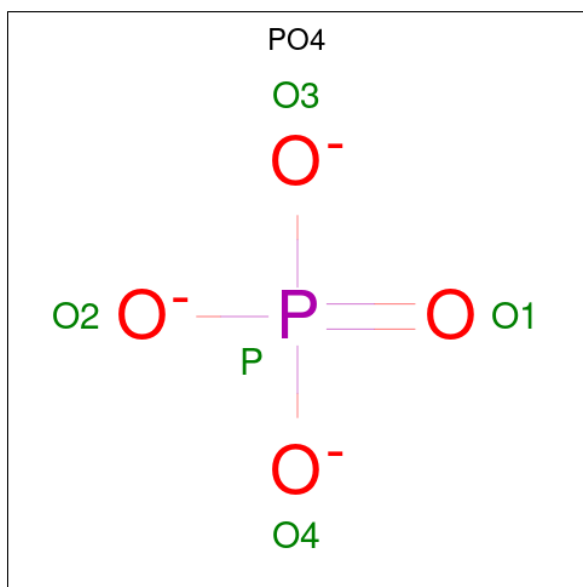
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	A	1	1	1	0	0
7	C	1	1	1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O P 5 4 1	0	0
9	C	1	Total O P 5 4 1	0	0
9	C	1	Total O P 5 4 1	0	0
9	E	1	Total O P 5 4 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	22	Total O 22 22	0	0
10	B	9	Total O 9 9	0	0
10	C	12	Total O 12 12	0	0
10	D	8	Total O 8 8	0	0

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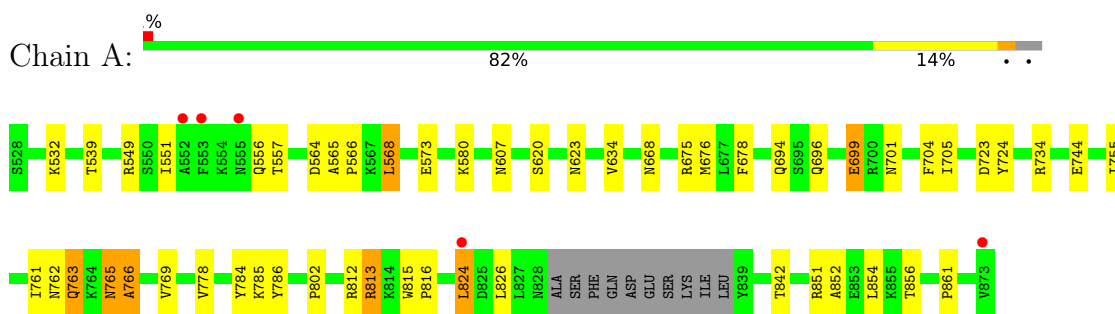
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	14	Total	O	0	0
			14	14		
10	F	6	Total	O	0	0
			6	6		

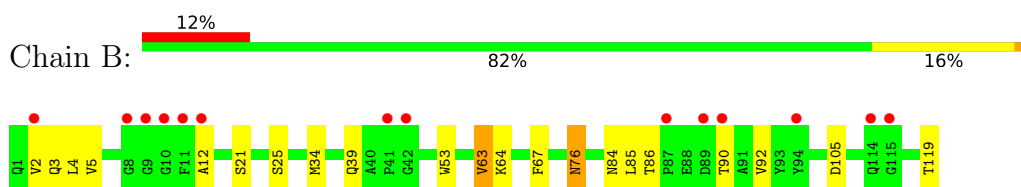
3 Residue-property plots [i](#)

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.

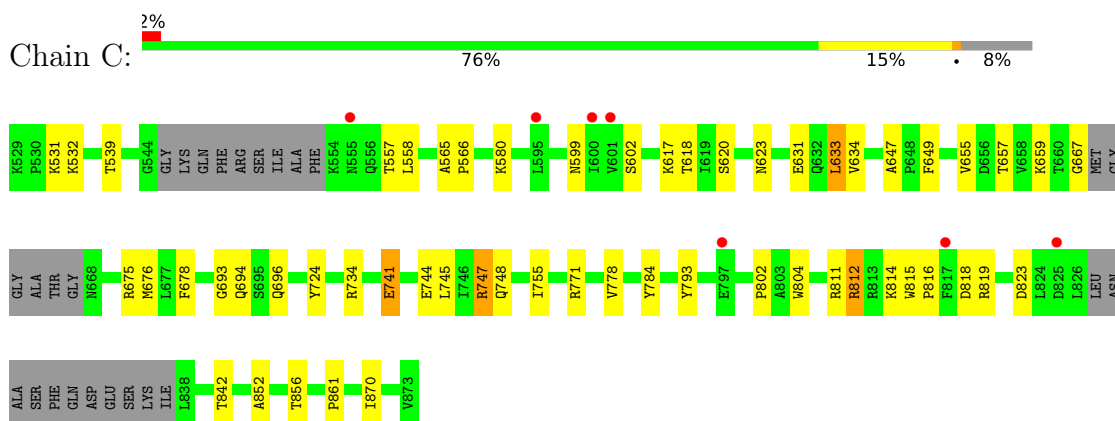
- Molecule 1: Isoform 2 of Synaptojanin-1



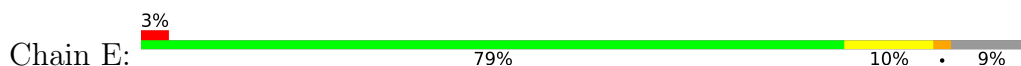
- Molecule 2: Nanobody 13015

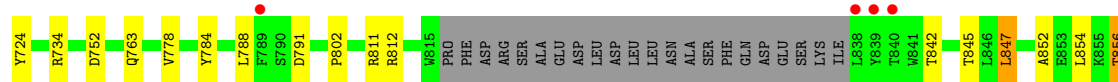


- Molecule 3: Isoform 2 of Synaptojanin-1

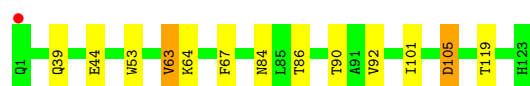
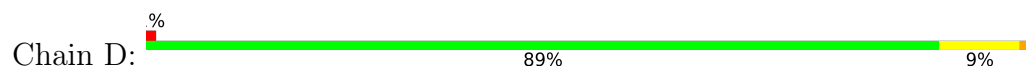


- Molecule 3: Isoform 2 of Synaptojanin-1

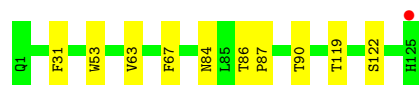
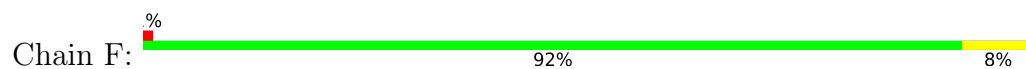




- Molecule 4: Nanobody 13015



- Molecule 5: Nanobody 13015



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.32Å 109.20Å 100.90Å 90.00° 120.62° 90.00°	Depositor
Resolution (Å)	87.39 – 2.73 87.39 – 2.73	Depositor EDS
% Data completeness (in resolution range)	76.2 (87.39-2.73) 70.0 (87.39-2.73)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.257 0.203 , 0.261	Depositor DCC
R_{free} test set	1629 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.017 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10780	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: IP9, PO4, MG, GOL

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	0.35	0/2775	0.64	2/3755 (0.1%)
2	B	0.33	0/915	0.61	0/1237
3	C	0.31	0/2641	0.60	0/3576
3	E	0.32	0/2595	0.61	0/3507
4	D	0.33	0/962	0.57	0/1298
5	F	0.34	0/981	0.60	0/1324
All	All	0.33	0/10869	0.61	2/14697 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	ALA	N-CA-CB	5.50	117.80	110.10
1	A	765	ASN	C-N-CA	5.21	134.72	121.70

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	2708	0	2671	28	0
2	B	896	0	821	10	0
3	C	2581	0	2528	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2537	0	2510	26	0
4	D	942	0	889	8	0
5	F	960	0	900	6	0
6	A	51	0	43	1	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	12	0	16	0	0
9	C	15	0	0	0	0
9	E	5	0	0	0	0
10	A	22	0	0	0	0
10	B	9	0	0	0	0
10	C	12	0	0	0	0
10	D	8	0	0	0	0
10	E	14	0	0	0	0
10	F	6	0	0	0	0
All	All	10780	0	10378	101	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 5.

All (101) 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:762:ASN:O	1:A:765:ASN:O	2.05	0.73
2:B:90:THR:HG22	2:B:119:THR:HA	1.69	0.73
1:A:668:ASN:ND2	6:A:901:IP9:O1P	2.20	0.72
3:E:724:TYR:CZ	3:E:812:ARG:HD2	2.24	0.72
4:D:105:ASP:N	4:D:105:ASP:OD1	2.23	0.70
1:A:724:TYR:CZ	1:A:812:ARG:HD2	2.27	0.69
3:E:592:MET:HA	3:E:592:MET:HE3	1.75	0.68
4:D:44:GLU:OE2	3:E:721:SER:HB3	1.94	0.67
3:C:744:GLU:O	3:C:747:ARG:HG2	1.96	0.64
1:A:696:GLN:HB3	1:A:699:GLU:HG2	1.79	0.64
3:C:694:GLN:HA	3:C:734:ARG:HG3	1.81	0.63
1:A:694:GLN:HA	1:A:734:ARG:HG3	1.82	0.62
3:C:565:ALA:HB3	3:C:566:PRO:HD3	1.82	0.61
3:E:633:LEU:HG	3:E:634:VAL:HG22	1.84	0.60
1:A:565:ALA:HB3	1:A:566:PRO:HD3	1.84	0.59
3:E:572:GLN:O	3:E:573:GLU:CB	2.50	0.58
3:C:744:GLU:HG3	3:C:748:GLN:NE2	2.19	0.58
5:F:63:VAL:HG13	5:F:67:PHE:CG	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:659:LYS:HG3	3:C:667:GLY:HA2	1.87	0.56
3:C:724:TYR:CZ	3:C:812:ARG:HD3	2.42	0.55
3:C:741:GLU:O	3:C:745:LEU:HD13	2.06	0.55
3:C:631:GLU:HB2	3:C:655:VAL:HG11	1.89	0.54
3:C:724:TYR:CE2	3:C:812:ARG:HD3	2.43	0.54
1:A:784:TYR:O	1:A:802:PRO:HA	2.07	0.54
4:D:44:GLU:OE2	3:E:721:SER:CB	2.56	0.54
1:A:824:LEU:C	1:A:824:LEU:HD23	2.28	0.53
3:E:784:TYR:O	3:E:802:PRO:HA	2.08	0.53
3:C:755:ILE:HD11	3:C:778:VAL:HB	1.90	0.53
3:C:784:TYR:O	3:C:802:PRO:HA	2.09	0.53
3:C:531:LYS:HE2	3:C:870:ILE:HD11	1.90	0.53
1:A:675:ARG:HG2	1:A:676:MET:N	2.25	0.52
3:C:793:TYR:CD2	3:C:802:PRO:HG3	2.44	0.52
1:A:551:ILE:N	1:A:551:ILE:HD12	2.25	0.51
3:E:675:ARG:HG2	3:E:676:MET:N	2.26	0.51
3:E:778:VAL:O	3:E:778:VAL:HG23	2.10	0.51
3:C:693:GLY:HA3	3:C:696:GLN:HE21	1.75	0.51
1:A:696:GLN:HB3	1:A:699:GLU:CG	2.41	0.51
1:A:778:VAL:O	1:A:778:VAL:HG23	2.11	0.50
2:B:84:ASN:HD22	2:B:84:ASN:N	2.10	0.49
3:E:552:ALA:HB1	3:E:856:THR:CG2	2.43	0.49
2:B:2:VAL:HG23	2:B:25:SER:O	2.13	0.49
3:C:558:LEU:HB2	3:C:618:THR:HG21	1.94	0.49
3:C:675:ARG:HG2	3:C:676:MET:N	2.26	0.49
2:B:76:ASN:N	2:B:76:ASN:HD22	2.10	0.48
1:A:620:SER:HA	1:A:623:ASN:O	2.14	0.47
3:E:847:LEU:HD13	3:E:847:LEU:N	2.29	0.47
1:A:826:LEU:HD22	1:A:826:LEU:N	2.30	0.47
3:E:653:VAL:HB	5:F:31:PHE:HB3	1.96	0.47
3:E:854:LEU:HD12	3:E:854:LEU:N	2.30	0.47
5:F:90:THR:HG23	5:F:119:THR:HA	1.96	0.47
3:C:620:SER:HA	3:C:623:ASN:O	2.15	0.47
4:D:90:THR:HG23	4:D:119:THR:HA	1.95	0.47
3:E:620:SER:HA	3:E:623:ASN:O	2.15	0.47
3:C:693:GLY:HA3	3:C:696:GLN:NE2	2.30	0.46
4:D:39:GLN:O	4:D:92:VAL:HG22	2.14	0.46
3:E:592:MET:HE3	3:E:592:MET:CA	2.45	0.46
5:F:87:PRO:HG3	5:F:122:SER:HA	1.98	0.46
1:A:701:ASN:HD21	1:A:763:GLN:CG	2.27	0.46
3:C:793:TYR:CE2	3:C:802:PRO:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:633:LEU:HD13	3:C:657:THR:HB	1.97	0.45
1:A:854:LEU:HD12	1:A:854:LEU:N	2.31	0.45
1:A:852:ALA:HB3	1:A:861:PRO:HG2	1.98	0.45
1:A:549:ARG:HE	1:A:607:ASN:HD21	1.65	0.45
1:A:784:TYR:HA	1:A:785:LYS:HA	1.81	0.45
3:E:552:ALA:HB1	3:E:856:THR:HG23	1.99	0.45
3:E:724:TYR:CE2	3:E:812:ARG:HD2	2.51	0.45
3:C:778:VAL:HG11	3:C:804:TRP:CE2	2.52	0.45
3:E:631:GLU:HB2	3:E:655:VAL:HG11	1.98	0.44
3:C:649:PHE:CE1	3:E:873:VAL:HB	2.53	0.44
5:F:86:THR:OG1	5:F:87:PRO:HD2	2.17	0.44
1:A:815:TRP:CE2	3:C:819:ARG:HG3	2.52	0.44
2:B:12:ALA:HB2	2:B:85:LEU:HD13	1.99	0.44
3:E:595:LEU:CD1	3:E:595:LEU:N	2.80	0.44
2:B:3:GLN:C	2:B:4:LEU:HD12	2.38	0.44
3:E:763:GLN:HA	3:E:763:GLN:OE1	2.18	0.44
3:C:599:ASN:HA	3:C:602:SER:O	2.18	0.43
4:D:44:GLU:CD	3:E:721:SER:HB3	2.38	0.43
3:E:852:ALA:HB3	3:E:861:PRO:HG2	2.00	0.43
1:A:704:PHE:HD2	1:A:705:ILE:HD12	1.83	0.43
2:B:39:GLN:O	2:B:92:VAL:HG12	2.18	0.43
3:C:814:LYS:NZ	3:C:818:ASP:OD1	2.51	0.43
3:E:788:LEU:HD22	3:E:788:LEU:H	1.83	0.43
3:C:815:TRP:CG	3:C:816:PRO:HD3	2.54	0.43
3:C:852:ALA:HB3	3:C:861:PRO:HG2	2.01	0.43
1:A:815:TRP:CG	1:A:816:PRO:HD3	2.54	0.43
2:B:5:VAL:O	2:B:5:VAL:HG13	2.18	0.43
1:A:701:ASN:HD21	1:A:763:GLN:HG3	1.84	0.42
1:A:723:ASP:HA	1:A:813:ARG:CD	2.48	0.42
5:F:63:VAL:HG13	5:F:67:PHE:HB2	2.01	0.42
2:B:4:LEU:HD12	2:B:4:LEU:N	2.34	0.42
1:A:786:TYR:OH	1:A:851:ARG:NH2	2.53	0.42
3:E:559:THR:HG21	3:E:621:ARG:NH1	2.34	0.42
3:E:845:THR:O	3:E:847:LEU:HD13	2.20	0.41
1:A:564:ASP:HB3	1:A:568:LEU:HD13	2.01	0.41
3:C:532:LYS:O	3:C:580:LYS:NZ	2.53	0.41
4:D:63:VAL:HG22	4:D:67:PHE:CG	2.55	0.41
2:B:63:VAL:HG22	2:B:67:PHE:CG	2.56	0.40
3:C:647:ALA:HA	4:D:101:ILE:HD11	2.04	0.40
3:C:815:TRP:N	3:C:816:PRO:CD	2.84	0.40
1:A:532:LYS:O	1:A:580:LYS:NZ	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ILE:HG23	1:A:761:ILE:HD13	2.03	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	333/346 (96%)	317 (95%)	14 (4%)	2 (1%)	25	44
2	B	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
3	C	311/345 (90%)	298 (96%)	11 (4%)	2 (1%)	25	44
3	E	305/345 (88%)	296 (97%)	7 (2%)	2 (1%)	22	40
4	D	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
5	F	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
All	All	1310/1403 (93%)	1266 (97%)	38 (3%)	6 (0%)	29	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	766	ALA
3	C	823	ASP
1	A	634	VAL
3	C	634	VAL
3	E	573	GLU
3	E	634	VAL

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	289/301 (96%)	275 (95%)	14 (5%)	25	44
2	B	87/93 (94%)	79 (91%)	8 (9%)	9	17
3	C	277/300 (92%)	265 (96%)	12 (4%)	29	48
3	E	272/300 (91%)	258 (95%)	14 (5%)	24	41
4	D	96/97 (99%)	90 (94%)	6 (6%)	18	31
5	F	98/99 (99%)	96 (98%)	2 (2%)	55	72
All	All	1119/1190 (94%)	1063 (95%)	56 (5%)	24	42

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	539	THR
1	A	556	GLN
1	A	557	THR
1	A	568	LEU
1	A	573	GLU
1	A	678	PHE
1	A	699	GLU
1	A	744	GLU
1	A	763	GLN
1	A	769	VAL
1	A	813	ARG
1	A	824	LEU
1	A	842	THR
1	A	856	THR
2	B	21	SER
2	B	34	MET
2	B	53	TRP
2	B	63	VAL
2	B	64	LYS
2	B	76	ASN
2	B	86	THR
2	B	105	ASP
3	C	539	THR
3	C	557	THR
3	C	617	LYS
3	C	633	LEU

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Mol	Chain	Res	Type
3	C	678	PHE
3	C	741	GLU
3	C	747	ARG
3	C	771	ARG
3	C	811	ARG
3	C	812	ARG
3	C	842	THR
3	C	856	THR
4	D	53	TRP
4	D	63	VAL
4	D	64	LYS
4	D	84	ASN
4	D	86	THR
4	D	105	ASP
3	E	539	THR
3	E	557	THR
3	E	592	MET
3	E	595	LEU
3	E	698	LYS
3	E	709	ARG
3	E	710	LYS
3	E	734	ARG
3	E	752	ASP
3	E	791	ASP
3	E	811	ARG
3	E	842	THR
3	E	847	LEU
3	E	856	THR
5	F	53	TRP
5	F	84	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	ASN
1	A	679	HIS
1	A	750	ASN
1	A	828	ASN
2	B	76	ASN
2	B	84	ASN
3	C	608	GLN
3	C	696	GLN

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Mol	Chain	Res	Type
3	C	748	GLN
3	C	859	HIS
3	E	632	GLN
3	E	679	HIS
3	E	750	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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
8	GOL	A	903	-	5,5,5	0.09	0	5,5,5	0.27	0
9	PO4	C	901	-	4,4,4	0.72	0	6,6,6	0.40	0
9	PO4	C	902	-	4,4,4	0.63	0	6,6,6	0.49	0
8	GOL	A	904	-	5,5,5	0.09	0	5,5,5	0.28	0
6	IP9	A	901	-	51,51,51	0.74	0	67,72,72	0.69	0
9	PO4	E	901	-	4,4,4	0.64	0	6,6,6	0.45	0
9	PO4	C	903	-	4,4,4	0.59	0	6,6,6	0.45	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
6	IP9	A	901	-	-	19/49/73/73	0/1/1/1
8	GOL	A	904	-	-	2/4/4/4	-
8	GOL	A	903	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

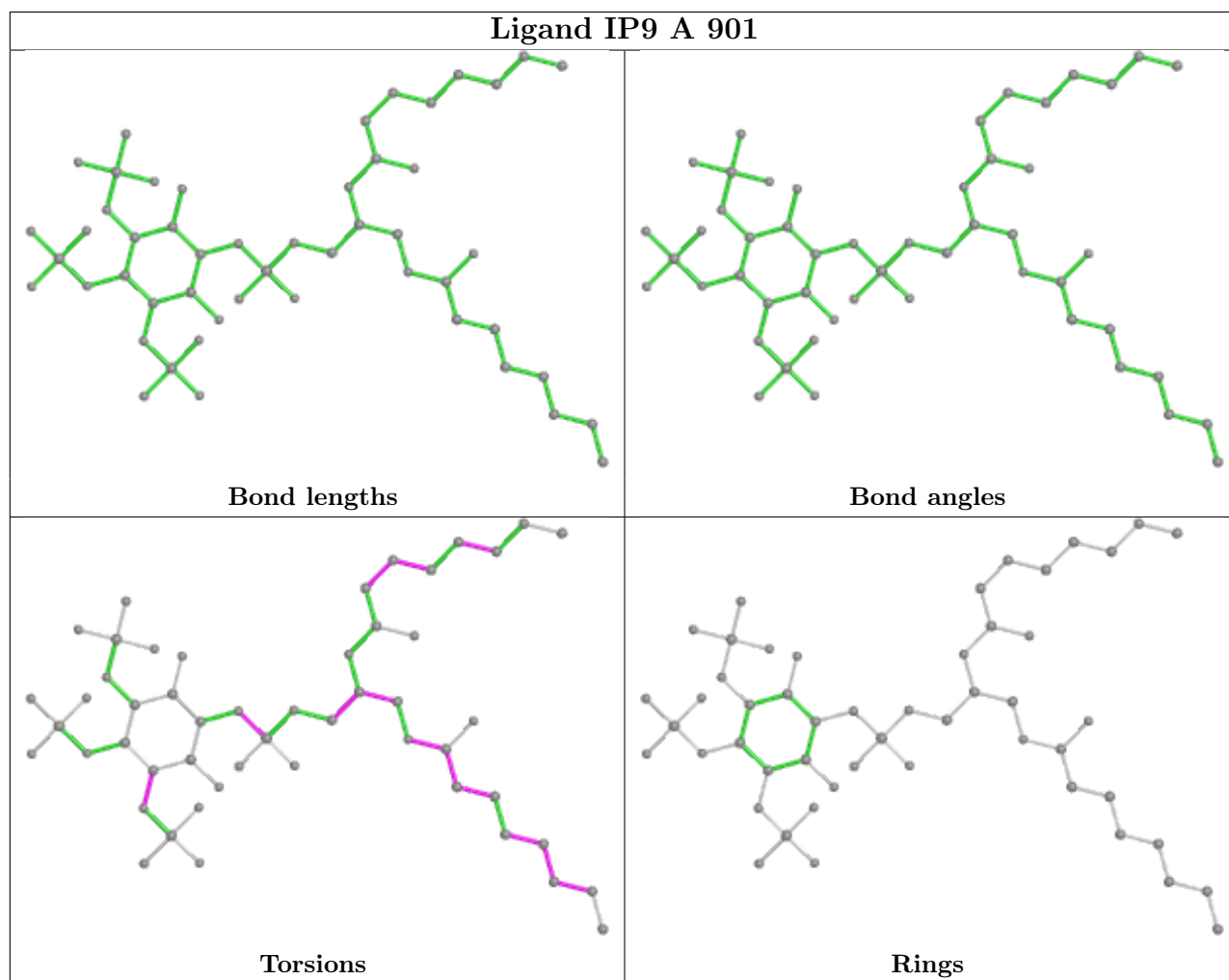
Mol	Chain	Res	Type	Atoms
6	A	901	IP9	C1-O1-P1-O2P
8	A	903	GOL	O1-C1-C2-O2
8	A	903	GOL	O1-C1-C2-C3
8	A	904	GOL	C1-C2-C3-O3
8	A	904	GOL	O2-C2-C3-O3
6	A	901	IP9	C13-C11-O20-C9
6	A	901	IP9	O22-C11-O20-C9
6	A	901	IP9	C10-C12-C14-C16
6	A	901	IP9	C11-C13-C15-C17
6	A	901	IP9	C7-C8-C9-O20
6	A	901	IP9	C16-C18-C20-C22
6	A	901	IP9	C1-O1-P1-O3P
6	A	901	IP9	C1-O1-P1-O1P
6	A	901	IP9	C17-C19-C21-C23
6	A	901	IP9	O19-C8-C9-O20
6	A	901	IP9	O3P-C7-C8-C9
6	A	901	IP9	O3P-C7-C8-O19
6	A	901	IP9	C15-C17-C19-C21
6	A	901	IP9	C19-C21-C23-C25
6	A	901	IP9	O20-C11-C13-C15
6	A	901	IP9	C2-C3-O3-P3
6	A	901	IP9	C12-C14-C16-C18
6	A	901	IP9	O22-C11-C13-C15

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	901	IP9	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.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	660:THR	C	667:GLY	N	5.44

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	336/346 (97%)	-0.10	5 (1%) 73 79	18, 31, 65, 102	0
2	B	119/119 (100%)	0.75	14 (11%) 4 4	28, 68, 99, 106	0
3	C	319/345 (92%)	-0.01	7 (2%) 62 69	26, 44, 80, 113	0
3	E	313/345 (90%)	0.12	9 (2%) 51 58	24, 45, 75, 107	0
4	D	123/123 (100%)	-0.09	1 (0%) 86 89	26, 38, 63, 80	0
5	F	125/125 (100%)	-0.16	1 (0%) 86 89	20, 32, 59, 95	0
All	All	1335/1403 (95%)	0.04	37 (2%) 53 60	18, 40, 83, 113	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	555	ASN	4.7
3	E	839	TYR	4.6
2	B	90	THR	4.5
1	A	873	VAL	3.9
3	E	662	MET	3.7
2	B	94	TYR	3.5
3	E	873	VAL	3.3
2	B	87	PRO	3.1
1	A	553	PHE	3.1
3	C	595	LEU	3.0
2	B	12	ALA	2.9
1	A	552	ALA	2.9
2	B	8	GLY	2.8
2	B	115	GLY	2.7
2	B	2	VAL	2.7
3	E	838	LEU	2.6
3	C	601	VAL	2.6
3	E	578	ARG	2.5
1	A	824	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	825	ASP	2.4
4	D	1	GLN	2.4
1	A	555	ASN	2.4
5	F	125	HIS	2.3
3	C	600	ILE	2.3
3	E	572	GLN	2.3
2	B	10	GLY	2.3
2	B	114	GLN	2.3
2	B	41	PRO	2.2
3	C	817	PHE	2.2
3	E	789	PHE	2.2
2	B	11	PHE	2.2
2	B	42	GLY	2.2
3	E	840	THR	2.2
3	E	661	GLY	2.1
3	C	797	GLU	2.1
2	B	9	GLY	2.0
2	B	89	ASP	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.

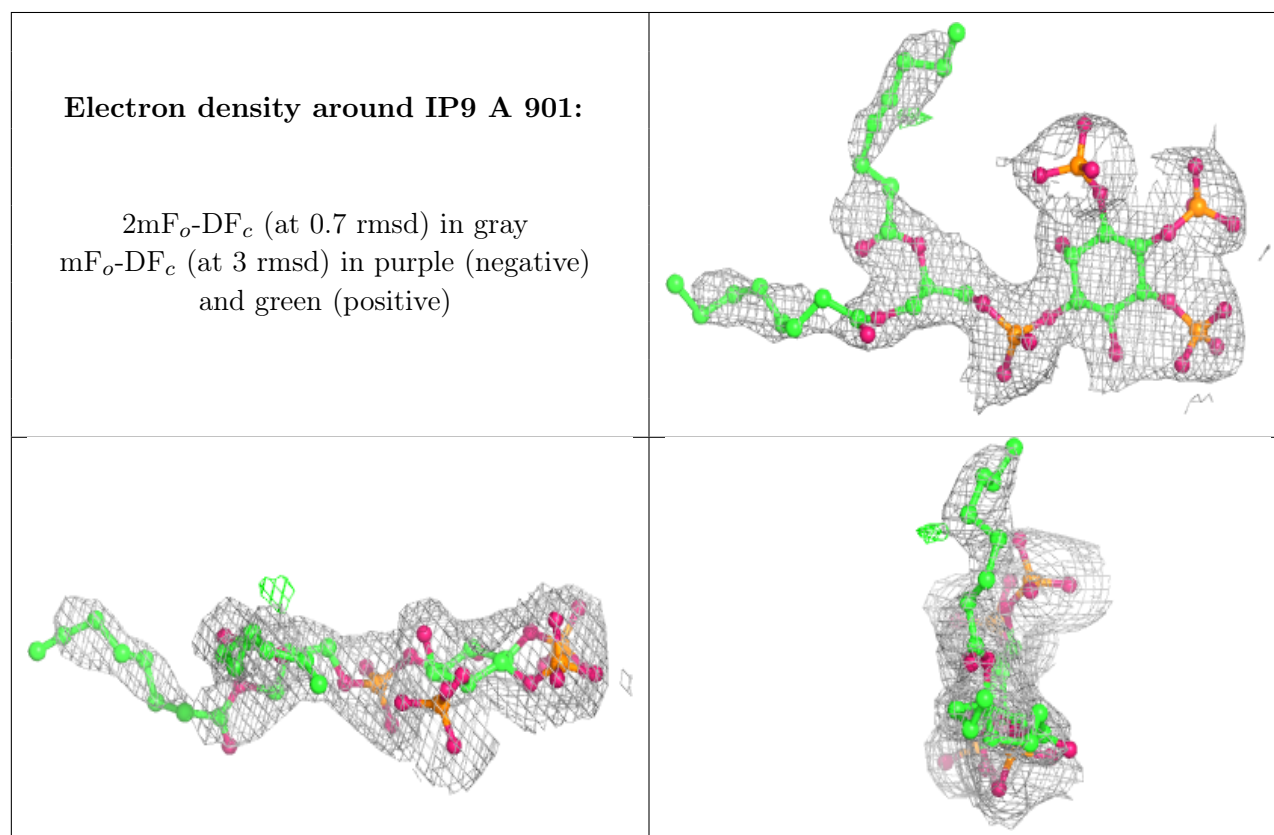
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	A	903	6/6	0.77	0.19	39,47,53,55	0
9	PO4	C	901	5/5	0.78	0.18	79,86,97,100	0
9	PO4	C	903	5/5	0.80	0.23	106,114,117,131	0
7	MG	A	902	1/1	0.85	0.17	46,46,46,46	0
9	PO4	E	901	5/5	0.88	0.18	80,82,95,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	A	904	6/6	0.91	0.14	35,42,49,54	0
7	MG	C	904	1/1	0.92	0.09	38,38,38,38	0
9	PO4	C	902	5/5	0.92	0.17	78,78,97,98	0
6	IP9	A	901	51/51	0.94	0.17	39,63,74,79	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.