Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 09:53 AM EDT

PDB ID	:	1Q6N
Title	:	THE STRUCTURE OF PHOSPHOTYROSINE PHOSPHATASE 1B IN COMPLEX WITH COMPOUND 4
Authors	:	Scapin, G.; Patel, S.B.; Becker, J.W.; Wang, Q.; Desponts, C.; Waddleton, D.; Skorey, K.; Cromlish, W.; Bayly, C.; Therien, M.; Gauthier, J.Y.; Li, C.S.; Lau, C.K.; Ramachandran, C.; Kennedy, B.P.; Asante-Appiah, E.
Deposited on	:	2003-08-13
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

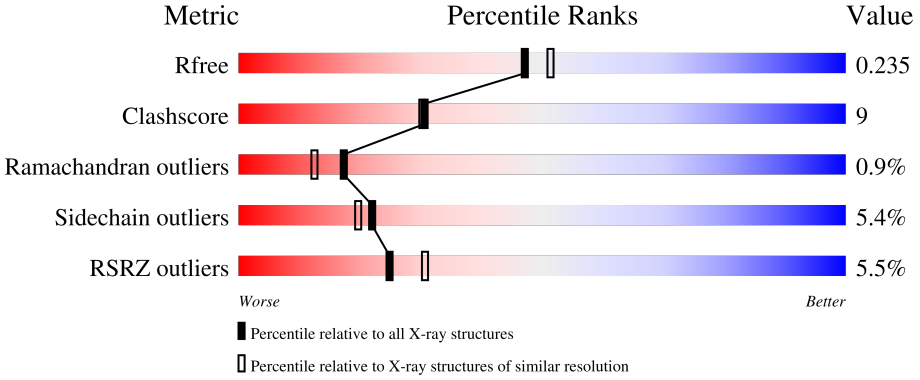
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	310	5%, 74%, 17%, • 7%
1	B	310	5%, 71%, 21%, • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5017 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 Protein-tyrosine phosphatase, non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2343	1484	404	439	16	0	0	0
1	B	289	2345	1488	404	437	16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	MET	-	cloning artifact	UNP P18031
A	490	ASP	-	cloning artifact	UNP P18031
A	491	TYR	-	cloning artifact	UNP P18031
A	492	LYS	-	cloning artifact	UNP P18031
A	493	ASP	-	cloning artifact	UNP P18031
A	494	ASP	-	cloning artifact	UNP P18031
A	495	ASP	-	cloning artifact	UNP P18031
A	496	ASP	-	cloning artifact	UNP P18031
A	497	LYS	-	cloning artifact	UNP P18031
A	498	LEU	-	cloning artifact	UNP P18031
A	499	GLU	-	cloning artifact	UNP P18031
A	500	PHE	-	cloning artifact	UNP P18031
B	989	MET	-	cloning artifact	UNP P18031
B	990	ASP	-	cloning artifact	UNP P18031
B	991	TYR	-	cloning artifact	UNP P18031
B	992	LYS	-	cloning artifact	UNP P18031
B	993	ASP	-	cloning artifact	UNP P18031
B	994	ASP	-	cloning artifact	UNP P18031
B	995	ASP	-	cloning artifact	UNP P18031
B	996	ASP	-	cloning artifact	UNP P18031
B	997	LYS	-	cloning artifact	UNP P18031
B	998	LEU	-	cloning artifact	UNP P18031
B	999	GLU	-	cloning artifact	UNP P18031
B	1000	PHE	-	cloning artifact	UNP P18031

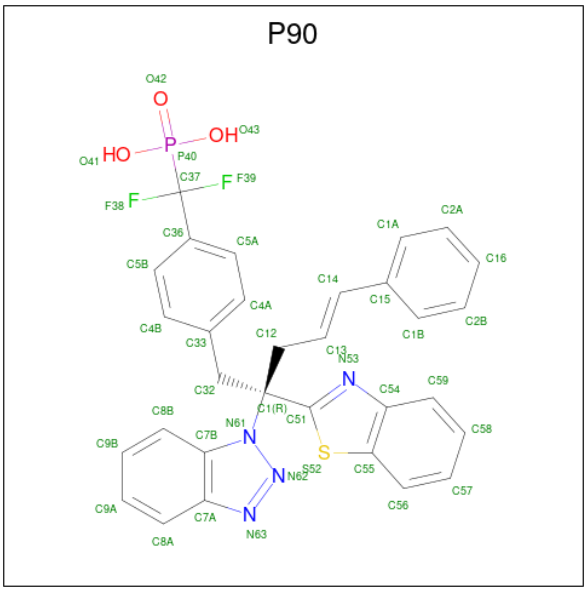
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is {4-[(2S,4E)-2-(1,3-BENZOTHIAZOL-2-YL)-2-(1H-1,2,3-BENZOTRIAZOL-1-YL)-5-PHENYLPENT-4-ENYL]PHENYL}(DIFLUORO)METHYLPHOSPHONIC ACID (three-letter code: P90) (formula: $C_{31}H_{25}F_2N_4O_3PS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O P S 42 31 2 4 3 1 1	0	0
4	B	1	Total C F N O P S 42 31 2 4 3 1 1	0	0

- Molecule 5 is water.

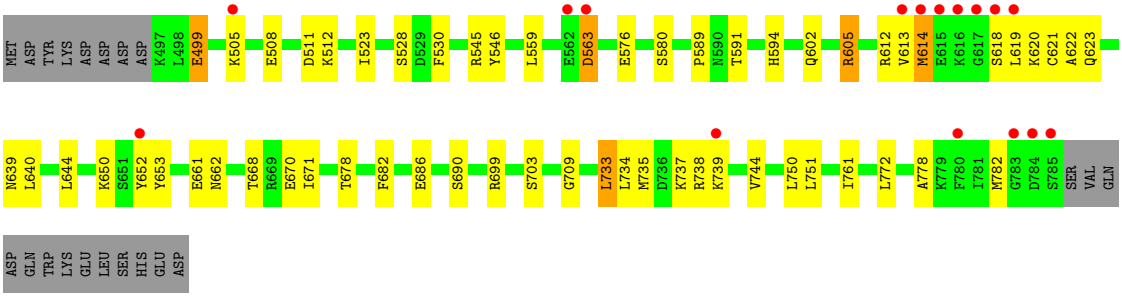
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	128	128	128	0	0
			Total	O		
5	B	111	111	111	0	0

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.

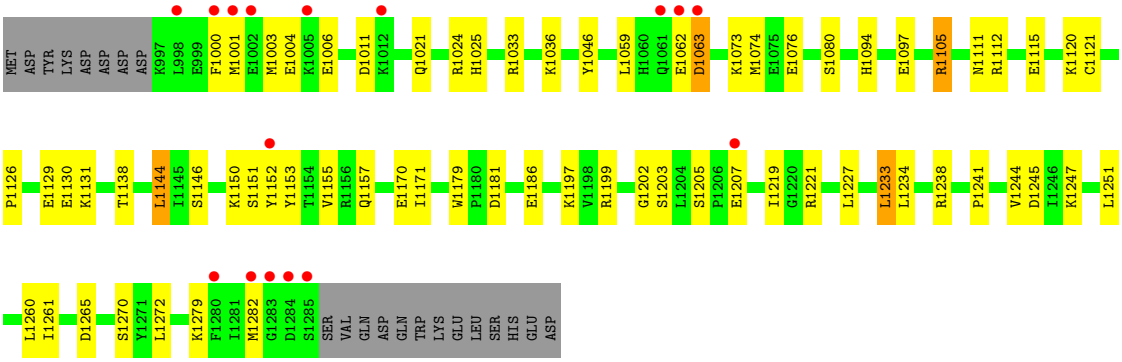
• Molecule 1: Protein-tyrosine phosphatase, non-receptor type 1

Chain A:



• Molecule 1: Protein-tyrosine phosphatase, non-receptor type 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.88Å 88.41Å 139.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 37.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (25.00-2.10) 92.8 (37.91-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.20 (at 2.00Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.208 , 0.238 0.206 , 0.235	Depositor DCC
R_{free} test set	2882 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.043 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5017	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: P90, CL, MG

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	0.69	0/2395	0.75	0/3228
1	B	0.64	0/2398	0.72	0/3232
All	All	0.67	0/4793	0.74	0/6460

There are no bond length outliers.

There are no bond angle outliers.

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	2343	0	2299	40	0
1	B	2345	0	2302	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	A	42	0	23	2	0
4	B	42	0	23	1	0
5	A	128	0	0	3	0
5	B	111	0	0	1	0
All	All	5017	0	4647	87	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 9.

All (87) 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:614:MET:HA	1:A:620:LYS:HB2	1.59	0.84
1:A:699:ARG:NH2	1:A:733:LEU:HD13	2.01	0.74
1:A:576:GLU:OE2	1:A:738:ARG:HD3	1.88	0.73
1:B:1024:ARG:HD2	3:B:6002:CL:CL	2.27	0.72
1:A:734:LEU:O	1:A:738:ARG:HG3	1.92	0.70
1:B:1036:LYS:HA	1:B:1036:LYS:HE2	1.73	0.69
1:A:612:ARG:HH21	1:A:678:THR:HA	1.59	0.66
1:A:671:ILE:N	1:A:671:ILE:HD12	2.09	0.66
5:A:836:HOH:O	1:B:1025:HIS:HD2	1.78	0.65
1:A:605:ARG:HG2	1:A:703:SER:HA	1.80	0.64
1:B:1199:ARG:NH2	1:B:1233:LEU:HD13	2.13	0.63
1:A:613:VAL:HG22	5:A:2096:HOH:O	1.98	0.62
1:B:1205:SER:OG	1:B:1207:GLU:HG2	2.00	0.62
1:B:1112:ARG:HH11	1:B:1112:ARG:HG3	1.65	0.61
1:B:1111:ASN:HD21	1:B:1121:CYS:HB2	1.65	0.60
1:A:512:LYS:O	1:A:512:LYS:HD2	2.01	0.60
1:B:1105:ARG:HH21	1:B:1170:GLU:HG2	1.66	0.59
1:B:1130:GLU:HG2	1:B:1131:LYS:HG2	1.85	0.59
1:A:576:GLU:O	1:A:737:LYS:HE3	2.05	0.57
4:A:801:P90:H14	1:B:1025:HIS:CE1	2.40	0.57
1:A:589:PRO:HG3	1:A:614:MET:HE1	1.86	0.57
1:A:589:PRO:HG3	1:A:614:MET:CE	2.36	0.56
1:A:614:MET:HE3	1:A:622:ALA:HA	1.89	0.54
1:A:614:MET:HG2	1:A:620:LYS:HD2	1.90	0.54
1:B:1046:TYR:HB3	4:B:1301:P90:N62	2.23	0.54
1:A:612:ARG:NH2	1:A:678:THR:HA	2.22	0.53
1:B:1115:GLU:HB2	1:B:1120:LYS:HG3	1.89	0.53
1:B:1150:LYS:HB2	1:B:1153:TYR:O	2.08	0.53
1:A:605:ARG:NH2	1:A:670:GLU:HG2	2.24	0.53
1:A:670:GLU:C	1:A:671:ILE:HD12	2.30	0.53
1:B:1105:ARG:HG2	1:B:1203:SER:HA	1.92	0.52
1:B:1238:ARG:NH2	1:B:1244:VAL:HA	2.24	0.52
1:A:505:LYS:HA	1:A:508:GLU:OE2	2.11	0.51
1:B:1000:PHE:CZ	1:B:1241:PRO:HG3	2.46	0.51
1:B:1076:GLU:OE2	1:B:1238:ARG:HD3	2.10	0.51
1:B:1155:VAL:HG21	1:B:1197:LYS:NZ	2.25	0.51
1:A:650:LYS:HD2	1:A:653:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:ALA:O	1:A:782:MET:HB2	2.11	0.50
1:B:1171:ILE:HD12	1:B:1171:ILE:N	2.26	0.49
1:B:1105:ARG:NH2	1:B:1170:GLU:HG2	2.26	0.49
1:B:1129:GLU:OE1	1:B:1129:GLU:N	2.38	0.49
1:A:545:ARG:NH2	1:A:621:CYS:HA	2.28	0.48
1:A:546:TYR:HB3	4:A:801:P90:N62	2.29	0.48
1:B:1001:MET:HA	1:B:1004:GLU:OE2	2.13	0.48
1:A:602:GLN:O	1:A:709:GLY:HA3	2.13	0.48
1:A:605:ARG:CG	1:A:703:SER:HA	2.44	0.48
1:B:1073:LYS:HD3	1:B:1074:MET:N	2.29	0.47
1:B:1073:LYS:HD3	1:B:1073:LYS:C	2.35	0.47
1:B:1131:LYS:HB2	5:B:2136:HOH:O	2.14	0.47
1:B:1202:GLY:O	1:B:1205:SER:HB3	2.14	0.47
1:B:1152:TYR:CD1	1:B:1153:TYR:HD2	2.33	0.47
1:B:1155:VAL:HG21	1:B:1197:LYS:HZ2	1.78	0.47
1:A:671:ILE:N	1:A:671:ILE:CD1	2.77	0.46
5:A:1316:HOH:O	1:B:1025:HIS:HE1	1.98	0.46
1:A:652:TYR:HB3	1:A:686:GLU:OE1	2.16	0.46
1:A:661:GLU:HB2	1:A:668:THR:HG22	1.97	0.46
1:B:1197:LYS:O	1:B:1197:LYS:HD3	2.16	0.45
1:A:735:MET:HG2	1:A:744:VAL:HG21	1.97	0.45
1:B:1004:GLU:OE1	1:B:1279:LYS:HE2	2.17	0.45
1:B:1112:ARG:HG3	1:B:1112:ARG:NH1	2.30	0.45
1:B:1245:ASP:OD1	1:B:1247:LYS:HB3	2.16	0.45
1:A:512:LYS:HD2	1:A:512:LYS:C	2.37	0.45
1:B:1205:SER:HG	1:B:1207:GLU:HG2	1.80	0.45
1:B:1146:SER:OG	1:B:1157:GLN:HB2	2.17	0.44
1:B:1234:LEU:O	1:B:1238:ARG:HG3	2.18	0.44
1:B:1179:TRP:CE2	1:B:1221:ARG:HG2	2.53	0.43
1:A:559:LEU:HD11	1:A:594:HIS:HB3	2.00	0.43
1:A:640:LEU:HD23	1:A:662:ASN:HA	2.01	0.43
1:A:613:VAL:HG11	1:A:623:GLN:OE1	2.19	0.43
1:B:1097:GLU:HB2	1:B:1138:THR:HG21	2.00	0.43
1:B:1219:ILE:O	1:B:1260:LEU:HA	2.18	0.43
1:A:682:PHE:CD1	1:B:1021:GLN:HG3	2.52	0.43
1:B:1000:PHE:HA	1:B:1003:MET:CE	2.48	0.43
1:A:614:MET:HA	1:A:621:CYS:H	1.84	0.42
1:B:1000:PHE:HA	1:B:1003:MET:HE3	2.02	0.42
1:B:1059:LEU:HD11	1:B:1094:HIS:HB3	2.02	0.42
1:A:523:ILE:HD13	1:A:750:LEU:HD23	2.02	0.42
1:A:528:SER:HB3	1:A:530:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1000:PHE:H	1:B:1000:PHE:HD1	1.68	0.41
1:A:614:MET:N	1:A:621:CYS:O	2.46	0.41
1:A:738:ARG:NH2	1:A:744:VAL:HA	2.35	0.41
1:A:499:GLU:O	1:A:499:GLU:OE1	2.38	0.41
1:A:591:THR:HA	1:A:594:HIS:CD2	2.55	0.40
1:B:1063:ASP:OD1	1:B:1063:ASP:N	2.53	0.40
1:B:1227:LEU:HD23	1:B:1270:SER:OG	2.22	0.40
1:B:1073:LYS:HG2	1:B:1080:SER:OG	2.21	0.40
1:B:1126:PRO:HB2	1:B:1144:LEU:HB2	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	287/310 (93%)	273 (95%)	11 (4%)	3 (1%)	15	11
1	B	287/310 (93%)	272 (95%)	13 (4%)	2 (1%)	22	18
All	All	574/620 (93%)	545 (95%)	24 (4%)	5 (1%)	17	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	563	ASP
1	A	614	MET
1	A	761	ILE
1	B	1063	ASP
1	B	1261	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	258/283 (91%)	244 (95%)	14 (5%)	22	20
1	B	258/283 (91%)	244 (95%)	14 (5%)	22	20
All	All	516/566 (91%)	488 (95%)	28 (5%)	22	20

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	499	GLU
1	A	511	ASP
1	A	563	ASP
1	A	580	SER
1	A	605	ARG
1	A	618	SER
1	A	619	LEU
1	A	639	ASN
1	A	644	LEU
1	A	690	SER
1	A	733	LEU
1	A	739	LYS
1	A	751	LEU
1	A	772	LEU
1	B	1006	GLU
1	B	1011	ASP
1	B	1033	ARG
1	B	1062	GLU
1	B	1105	ARG
1	B	1144	LEU
1	B	1151	SER
1	B	1181	ASP
1	B	1186	GLU
1	B	1233	LEU
1	B	1251	LEU
1	B	1265	ASP
1	B	1272	LEU

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Mol	Chain	Res	Type
1	B	1282	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	525	HIS
1	A	561	GLN
1	A	594	HIS
1	A	639	ASN
1	B	1021	GLN
1	B	1025	HIS
1	B	1060	HIS
1	B	1094	HIS
1	B	1139	ASN
1	B	1157	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
4	P90	B	1301	-	39,47,47	2.78	26 (66%)	48,70,70	1.68	5 (10%)
4	P90	A	801	-	39,47,47	2.82	22 (56%)	48,70,70	1.62	6 (12%)

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
4	P90	B	1301	-	-	3/22/39/39	0/6/6/6
4	P90	A	801	-	-	1/22/39/39	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	P90	C32-C1	8.34	1.65	1.55
4	B	1301	P90	C32-C1	7.97	1.64	1.55
4	A	801	P90	C12-C1	4.99	1.60	1.55
4	B	1301	P90	C5A-C36	4.44	1.46	1.39
4	A	801	P90	N62-N61	4.12	1.42	1.34
4	B	1301	P90	C12-C1	4.04	1.59	1.55
4	A	801	P90	C9A-C8A	4.00	1.45	1.36
4	A	801	P90	C58-C59	3.75	1.45	1.36
4	B	1301	P90	N62-N61	3.71	1.41	1.34
4	B	1301	P90	C9A-C8A	3.59	1.44	1.36
4	A	801	P90	C57-C56	3.59	1.44	1.36
4	A	801	P90	C8B-C7B	3.50	1.48	1.41
4	A	801	P90	C9B-C8B	3.44	1.44	1.36
4	A	801	P90	C5A-C36	3.32	1.44	1.39
4	A	801	P90	C4A-C33	3.29	1.45	1.38
4	B	1301	P90	P40-O43	-3.26	1.48	1.54
4	B	1301	P90	C57-C56	3.19	1.44	1.36
4	A	801	P90	C5B-C36	3.17	1.44	1.39
4	B	1301	P90	P40-O42	-3.16	1.45	1.50
4	B	1301	P90	C8B-C7B	3.13	1.47	1.41
4	B	1301	P90	C37-C36	-3.07	1.48	1.50
4	A	801	P90	C5B-C4B	3.04	1.44	1.38
4	A	801	P90	C4B-C33	2.97	1.45	1.38
4	B	1301	P90	C9B-C8B	2.96	1.43	1.36
4	A	801	P90	N63-N62	2.94	1.39	1.34
4	B	1301	P90	C58-C59	2.91	1.43	1.36
4	B	1301	P90	C4B-C33	2.90	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	P90	C9B-C9A	2.88	1.45	1.38
4	B	1301	P90	P40-O41	-2.75	1.49	1.54
4	B	1301	P90	C51-S52	2.70	1.81	1.73
4	B	1301	P90	C5B-C36	2.68	1.43	1.39
4	A	801	P90	C2B-C1B	2.64	1.44	1.38
4	A	801	P90	C9B-C9A	2.62	1.44	1.38
4	B	1301	P90	C1B-C15	2.60	1.44	1.39
4	B	1301	P90	N63-N62	2.60	1.39	1.34
4	B	1301	P90	C58-C57	2.56	1.44	1.38
4	A	801	P90	C58-C57	2.48	1.44	1.38
4	B	1301	P90	C2B-C1B	2.48	1.44	1.38
4	B	1301	P90	C16-C2A	2.46	1.44	1.38
4	B	1301	P90	C4A-C33	2.41	1.44	1.38
4	A	801	P90	C1B-C15	2.36	1.44	1.39
4	A	801	P90	C16-C2A	2.36	1.44	1.38
4	B	1301	P90	C16-C2B	2.33	1.44	1.38
4	B	1301	P90	C32-C33	2.30	1.55	1.51
4	A	801	P90	C2A-C1A	2.26	1.43	1.38
4	A	801	P90	C16-C2B	2.23	1.43	1.38
4	A	801	P90	P40-O43	-2.14	1.50	1.54
4	B	1301	P90	C5B-C4B	2.04	1.42	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1301	P90	C7B-C7A-N63	-6.31	100.71	108.58
4	A	801	P90	C7B-C7A-N63	-5.75	101.40	108.58
4	B	1301	P90	C8A-C7A-N63	4.56	137.61	130.19
4	A	801	P90	C8A-C7A-N63	4.38	137.32	130.19
4	B	1301	P90	C8B-C7B-N61	-4.37	127.89	131.93
4	A	801	P90	C8B-C7B-N61	-3.51	128.69	131.93
4	A	801	P90	F38-C37-C36	-3.32	106.21	110.49
4	A	801	P90	P40-C37-C36	2.37	116.08	108.95
4	B	1301	P90	F39-C37-C36	-2.29	107.54	110.49
4	A	801	P90	C1-C12-C13	-2.09	110.50	114.12
4	B	1301	P90	C12-C13-C14	-2.03	120.81	123.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	P90	C1-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	B	1301	P90	C1-C12-C13-C14
4	B	1301	P90	C13-C14-C15-C1B
4	B	1301	P90	C13-C14-C15-C1A

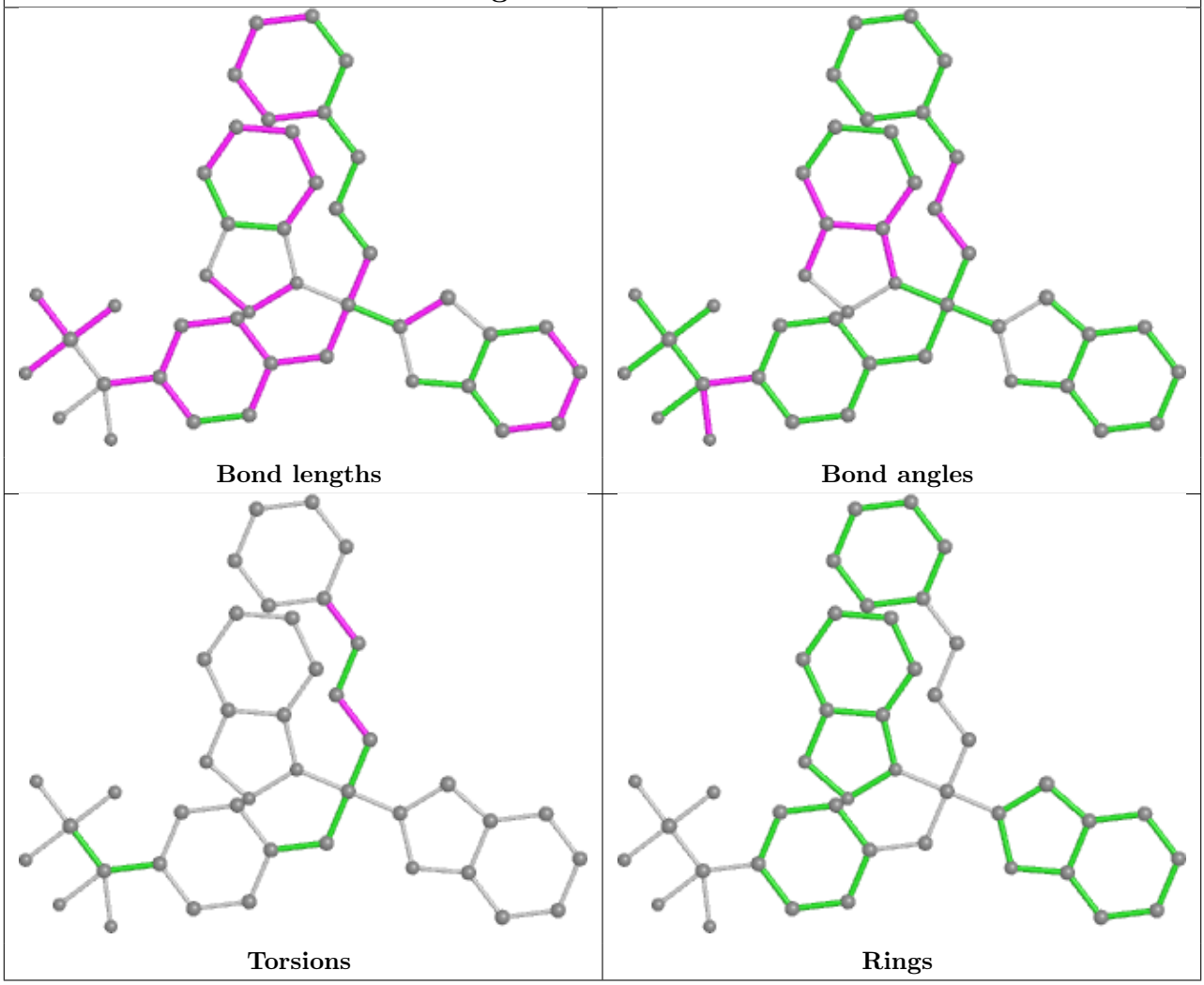
There are no ring outliers.

2 monomers are involved in 3 short contacts:

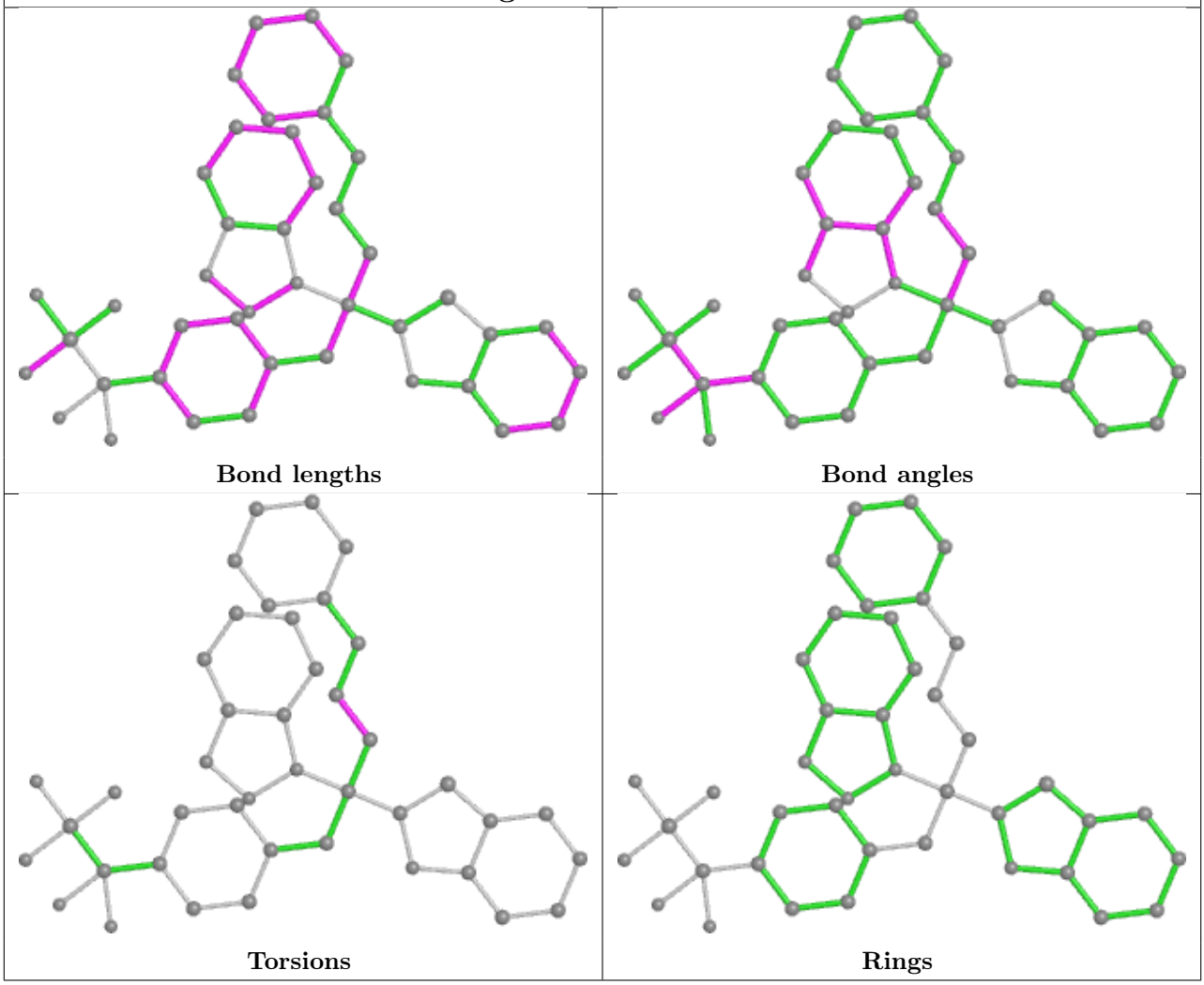
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1301	P90	1	0
4	A	801	P90	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 P90 B 1301



Ligand P90 A 801



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	289/310 (93%)	-0.04	16 (5%)	25	31	18, 30, 66, 83	0
1	B	289/310 (93%)	0.09	16 (5%)	25	31	16, 37, 63, 84	0
All	All	578/620 (93%)	0.03	32 (5%)	25	31	16, 33, 65, 84	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	617	GLY	7.5
1	A	785	SER	6.8
1	A	616	LYS	6.2
1	B	1285	SER	5.7
1	A	784	ASP	5.5
1	B	1284	ASP	5.0
1	B	998	LEU	4.9
1	A	614	MET	4.8
1	B	1000	PHE	4.6
1	B	1005	LYS	4.3
1	B	1002	GLU	4.0
1	B	1062	GLU	3.7
1	A	783	GLY	3.5
1	A	563	ASP	3.4
1	A	618	SER	3.2
1	A	619	LEU	3.2
1	B	1282	MET	3.1
1	A	615	GLU	3.1
1	A	780	PHE	3.1
1	B	1001	MET	3.1
1	B	1280	PHE	3.0
1	B	1283	GLY	2.9
1	B	1061	GLN	2.8
1	B	1152	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	613	VAL	2.5
1	B	1012	LYS	2.5
1	A	505	LYS	2.4
1	A	562	GLU	2.3
1	A	739	LYS	2.3
1	A	652	TYR	2.3
1	B	1063	ASP	2.2
1	B	1207	GLU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

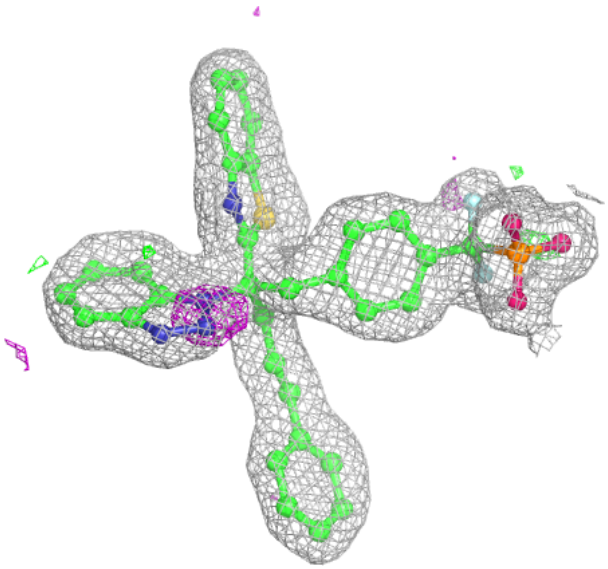
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

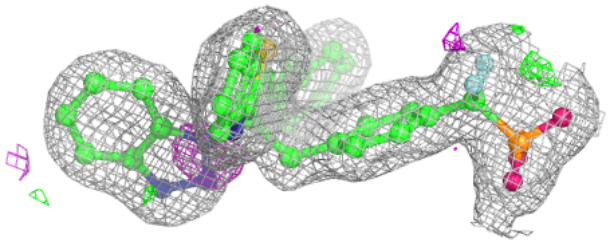
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	5000	1/1	0.91	0.14	45,45,45,45	1
2	MG	B	5030	1/1	0.91	0.28	43,43,43,43	1
2	MG	B	5020	1/1	0.93	0.06	43,43,43,43	1
2	MG	A	5010	1/1	0.95	0.05	42,42,42,42	1
4	P90	A	801	42/42	0.96	0.12	19,24,31,32	0
4	P90	B	1301	42/42	0.98	0.12	19,28,32,33	0
3	CL	A	6001	1/1	0.99	0.05	26,26,26,26	0
3	CL	B	6002	1/1	1.00	0.09	26,26,26,26	0

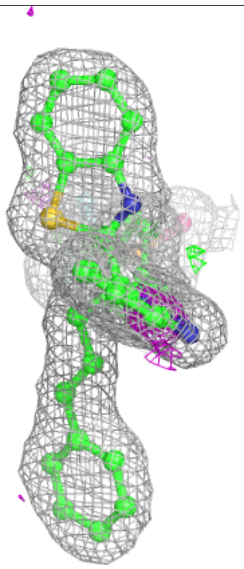
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P90 A 801:

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

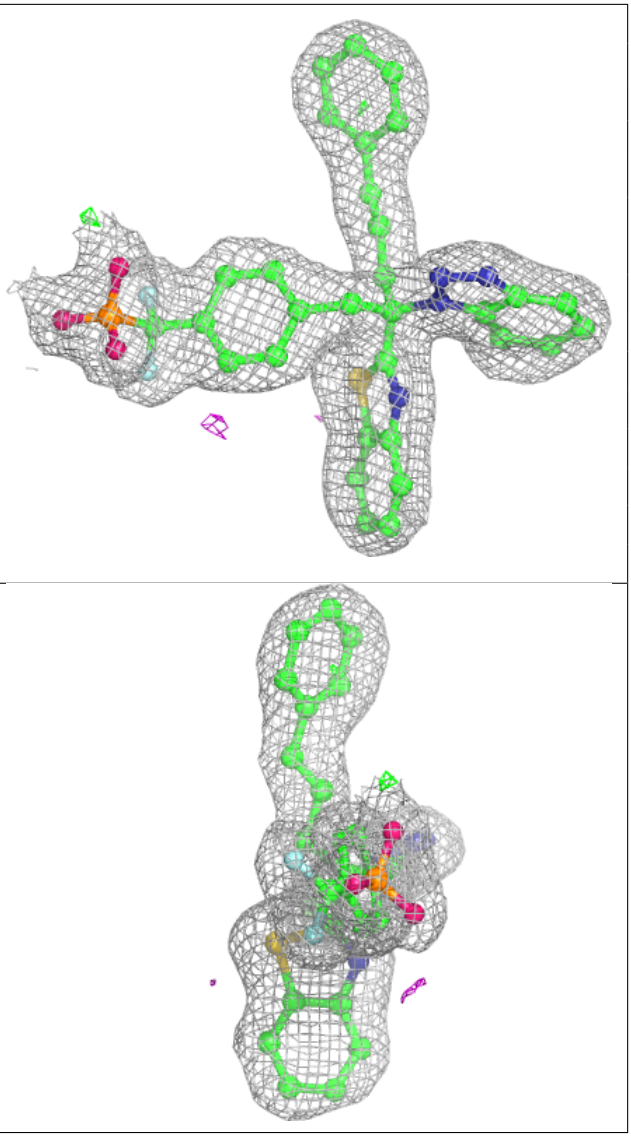






Electron density around P90 B 1301:

$2mF_o$-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.