



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:26 PM BST

PDB ID : 3U17
Title : Structure of BasE N-terminal domain from *Acinetobacter baumannii* bound to 6-(p-benzoyl)phenyl-1-(pyridin-4-ylmethyl)-1H-pyrazolo[3,4-b]pyridine-4-carboxylic acid
Authors : Gulick, A.M.; Drake, E.J.; Aldrich, C.C.; Neres, J.
Deposited on : 2011-09-29
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

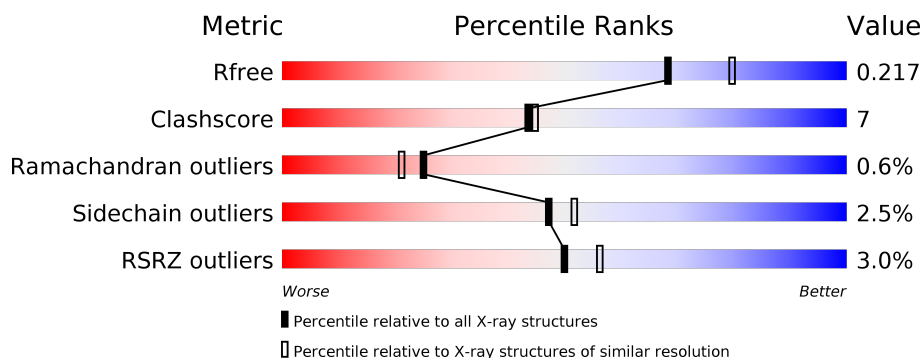
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 on 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	544	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>10%</div> <div>20%</div> </div> </div>
1	B	544	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>12%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7241 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.

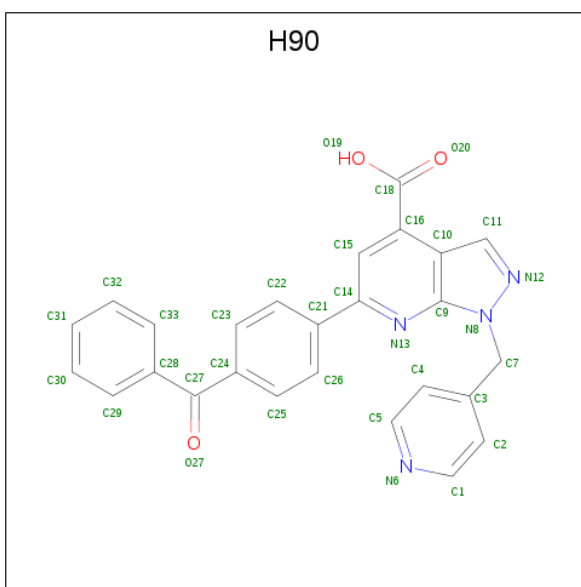
- Molecule 1 is a protein called Peptide arylation enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	2	0
			3382	2152	581	634	15			
1	B	436	Total	C	N	O	S	0	1	0
			3389	2160	574	640	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B2HVG8
A	0	HIS	-	expression tag	UNP B2HVG8
A	45	LEU	PRO	SEE REMARK 999	UNP B2HVG8
A	68	THR	SER	SEE REMARK 999	UNP B2HVG8
A	149	ASP	GLU	SEE REMARK 999	UNP B2HVG8
A	180	PHE	LEU	SEE REMARK 999	UNP B2HVG8
A	226	GLY	ASP	SEE REMARK 999	UNP B2HVG8
A	329	LEU	ILE	SEE REMARK 999	UNP B2HVG8
A	378	ARG	LYS	SEE REMARK 999	UNP B2HVG8
B	-1	GLY	-	expression tag	UNP B2HVG8
B	0	HIS	-	expression tag	UNP B2HVG8
B	45	LEU	PRO	SEE REMARK 999	UNP B2HVG8
B	68	THR	SER	SEE REMARK 999	UNP B2HVG8
B	149	ASP	GLU	SEE REMARK 999	UNP B2HVG8
B	180	PHE	LEU	SEE REMARK 999	UNP B2HVG8
B	226	GLY	ASP	SEE REMARK 999	UNP B2HVG8
B	329	LEU	ILE	SEE REMARK 999	UNP B2HVG8
B	378	ARG	LYS	SEE REMARK 999	UNP B2HVG8

- Molecule 2 is 6-(4-benzoylphenyl)-1-(pyridin-4-ylmethyl)-1H-pyrazolo[3,4-b]pyridine-4-carboxylic acid (three-letter code: H90) (formula: C₂₆H₁₈N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	26	4	3		
2	B	1	Total	C	N	O	0	0
			33	26	4	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

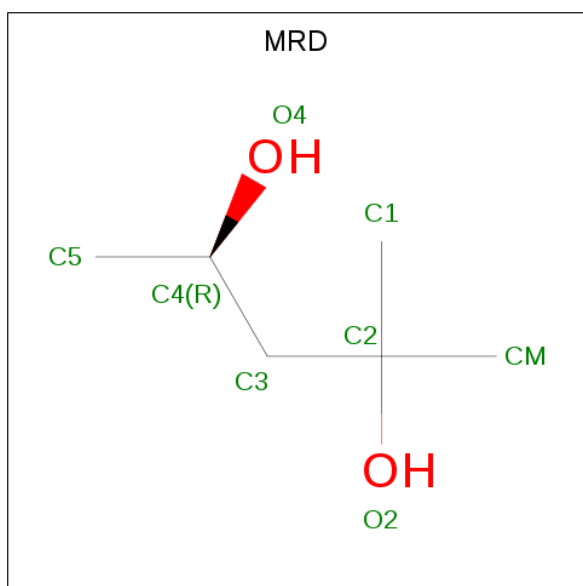
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	4	Total	Ca	0	0
			4	4		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	184	Total 184	O 184	0	0
6	B	197	Total 197	O 197	0	0

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.

Chain A:

3% 68% 10% 20%

GLY HIS MET LYS K3 R15 Y19 D27 V38 H41 P42 H43 S44 T64 I65 L66 A67 T68 A69 L70 K73 G74 L75 L106 Q114 Y115 M118 Q125 R133 Q134 H135 E136 V137 F138 S139 F143 I144 D149 V150 H151 L152 I156 M161 H162

Q163 A164 D166 F167 T175 P176 A177 E178 T179 F180 V181 Q196 L196 S197 G198 GLY T201 G202 T203 N212 D213 E223 N228 S229 N230 C235 A239 P240 P248 V260 N265 P266 E267 P268 T291 E295 Q305 Q311 G314 N330 C342 C343

LYS SER CYS ALA PHE ILE VAL SER ARG ASN PRO GLU LEU LYS ALA VAL LEU ARG HIS LEU MET GLU GLY ILE ALA GLN TYR LYS LEU PRO ASP GLN ILE LYS LEU ILE GLU SER LEU PRO LEU THR VAL VAL GLY LYS VAL ASP VAL LYS LYS GLN LEU ARG SER ILE LEU LEU

THR SER THR THR SER

Chain B:

Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.10). The x-axis lists amino acids. A bar chart at the top shows the percentage of each amino acid in the sequence: 2% (red), 67% (green), 12% (yellow), and 20% (grey).

Position	Amino Acid	Information Content (bits)
1	GLY	0.08
2	HIS	0.02
3	MET	0.02
4	LYS	0.02
5	K3	0.02
6	D27	0.02
7	V38	0.02
8	Q39	0.02
9	P42	0.02
10	H43	0.02
11	S44	0.02
12	R52	0.02
13	L62	0.02
14	N65	0.02
15	R69	0.02
16	E72	0.02
17	K77	0.02
18	E90	0.02
19	L98	0.02
20	V105	0.02
21	R133	0.02
22	Q134	0.02
23	H135	0.02
24	E136	0.02
25	V137	0.02
26	H148	0.02
27	D149	0.02
28	V150	0.02
29	H162	0.02
30	Q163	0.02
31	D166	0.02
32	L170	0.02
33	I173	0.02
34	E174	0.02
35	T175	0.02
36	P176	0.02
37	A177	0.02
38	E178	0.02
39	T179	0.02
40	F180	0.02
41	S195	0.02
42	F193	0.02
43	Q195	0.02
44	L196	0.02
45	G199	0.02
46	S200	0.02
47	T201	0.02
48	N212	0.02
49	D213	0.02
50	H214	0.02
51	D215	0.02
52	R219	0.02
53	C225	0.02
54	G226	0.02
55	L233	0.02
56	L234	0.02
57	C235	0.02
58	P248	0.02
59	V253	0.02
60	V260	0.02
61	N265	0.02
62	P266	0.02
63	E267	0.02
64	P268	0.02
65	L269	0.02
66	N270	0.02
67	C271	0.02
68	V280	0.02
69	T291	0.02
70	E295	0.02
71	Q311	0.02
72	G314	0.02
73	A315	0.02
74	G342	0.02
75	R348	0.02
76	R362	0.02
77	E369	0.02
78	I370	0.02
79	F180	0.02
80	K371	0.02
81	E382	0.02
82	R391	0.02
83	Y394	0.02
84	T395	0.02
85	F396	0.02
86	E404	0.02
87	Q408	0.02
88	Y415	0.02
89	T425	0.02
90	P426	0.02
91	V433	0.02
92	K437	0.02
93	D438	0.02
94	GLN	0.02
95	ILE	0.02
96	ASN	0.02
97	GLU	0.02
98	LEU	0.02
99	ILE	0.02
100	GLY	0.02
101	ILE	0.02
102	ALA	0.02
103	GLN	0.02
104	TYR	0.02
105	LYS	0.02
106	LEU	0.02
107	SER	0.02
108	GLU	0.02
109	ASP	0.02
110	ILE	0.02
111	GLU	0.02
112	LYS	0.02
113	LEU	0.02
114	ILE	0.02
115	LEU	0.02
116	SER	0.02
117	LEU	0.02
118	PRO	0.02
119	LEU	0.02
120	THR	0.02
121	ALA	0.02
122	VAL	0.02
123	HIS	0.02
124	ALA	0.02
125	LYS	0.02
126	ASP	0.02
127	VAL	0.02
128	GLN	0.02
129	LEU	0.02
130	ARG	0.02
131	ILE	0.02
132	PHE	0.02
133	GLY	0.02
134	LEU	0.02
135	ASN	0.02
136	THR	0.02
137	SER	0.02
138	THR	0.02
139	THR	0.02
140	SER	0.02

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.37Å 144.23Å 148.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 45.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.1 (40.00-2.10) 90.1 (45.75-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2), REFMAC (Diff. Fourier)	Depositor
R, R_{free}	0.189 , 0.221 0.185 , 0.217	Depositor DCC
R_{free} test set	3724 reflections (4.99%)	wwPDB-VI
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7241	wwPDB-VI
Average B, all atoms (Å ²)	41.0	wwPDB-VI

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: H90, MRD, CA, MPD

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	0.37	0/3461	0.52	0/4711
1	B	0.37	0/3471	0.51	0/4728
All	All	0.37	0/6932	0.51	0/9439

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

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	3382	0	3302	45	0
1	B	3389	0	3292	44	0
2	A	33	0	17	3	0
2	B	33	0	17	2	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
4	A	8	0	14	1	0
5	B	8	0	14	0	0
6	A	184	0	0	3	0
6	B	197	0	0	1	0
All	All	7241	0	6656	91	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 7.

All (91) 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:305[A]:GLN:HE22	1:A:330:ASN:HD22	1.11	0.94
1:A:401:GLN:HG2	6:A:585:HOH:O	1.72	0.88
1:A:106:LEU:HD11	1:A:196:LEU:HD21	1.63	0.81
1:B:269:LEU:H	1:B:269:LEU:HD12	1.48	0.79
1:A:228:ASN:HD22	1:A:230:ASN:H	1.30	0.78
1:A:352:SER:H	1:A:355:GLN:HE21	1.31	0.78
1:B:248:PRO:HD3	1:B:311:GLN:HE22	1.50	0.77
1:B:248:PRO:HD3	1:B:311:GLN:NE2	2.04	0.72
1:B:213:ASP:HB2	1:B:394:TYR:HA	1.72	0.71
1:A:228:ASN:ND2	1:A:230:ASN:H	1.90	0.68
1:A:235[B]:CYS:SG	1:A:260:VAL:HG13	2.33	0.67
1:A:195:GLN:HE21	1:A:196:LEU:H	1.44	0.66
1:B:235[B]:CYS:SG	1:B:260:VAL:HG13	2.38	0.62
1:A:213:ASP:HB2	1:A:394:TYR:HA	1.82	0.61
1:B:90:GLU:OE2	1:B:170:LEU:HD21	2.00	0.61
1:B:269:LEU:H	1:B:269:LEU:CD1	2.14	0.61
1:B:133:ARG:HG3	1:B:163:GLN:HG2	1.84	0.60
1:B:200:SER:HB3	6:B:584:HOH:O	1.99	0.60
1:B:225:CYS:SG	1:B:248:PRO:HG3	2.45	0.57
1:B:174:GLU:HG2	1:B:175:THR:HG23	1.87	0.56
1:A:15:ARG:HD2	1:A:19:TYR:OH	2.06	0.55
1:A:228:ASN:HD22	1:A:228:ASN:C	2.10	0.55
1:B:269:LEU:HD12	1:B:269:LEU:N	2.20	0.55
1:A:64:THR:O	1:A:68:THR:HG23	2.07	0.53
1:B:38:VAL:O	1:B:42:PRO:HG3	2.08	0.53
2:A:543:H90:C9	2:A:543:H90:H2	2.37	0.53
1:B:72:GLU:OE1	1:B:177:ALA:HB1	2.08	0.53
1:B:265:ASN:HB2	1:B:266:PRO:CD	2.38	0.52
1:A:352:SER:H	1:A:355:GLN:NE2	2.04	0.52
1:B:348:ARG:HG2	1:B:362:ARG:NH2	2.26	0.51
1:B:314:GLY:HA2	2:B:543:H90:C10	2.40	0.51
1:B:437:LYS:N	1:B:437:LYS:HD3	2.26	0.51
1:B:65:ASN:O	1:B:69:ARG:HG2	2.11	0.50
2:B:543:H90:C9	2:B:543:H90:H2	2.41	0.50
1:B:135:HIS:CE1	1:B:137:VAL:HG23	2.47	0.50
1:A:115:TYR:OH	1:B:291:ILE:HG22	2.12	0.50
1:B:267:GLU:HB3	1:B:269:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:O	1:A:166:ASP:HB2	2.12	0.49
1:A:144:ILE:HG12	6:A:715:HOH:O	2.12	0.49
1:A:291:ILE:O	1:A:295:GLU:HG2	2.13	0.49
1:B:235[B]:CYS:SG	1:B:260:VAL:CG1	3.01	0.49
1:B:266:PRO:HA	1:B:271:CYS:SG	2.53	0.48
1:A:228:ASN:HD22	1:A:230:ASN:N	2.05	0.48
1:A:305[A]:GLN:NE2	1:A:330:ASN:HD22	1.94	0.47
1:A:248:PRO:HD3	1:A:311:GLN:NE2	2.30	0.47
1:A:118:ASN:ND2	1:A:143:PHE:HE1	2.13	0.47
1:B:233:LEU:HB3	1:B:253:VAL:HG21	1.96	0.47
1:B:135:HIS:HE1	1:B:137:VAL:HG23	1.80	0.47
1:B:234:LEU:HB2	1:B:280:VAL:HG11	1.97	0.47
1:A:235[B]:CYS:SG	1:A:260:VAL:CG1	3.04	0.46
1:A:38:VAL:O	1:A:42:PRO:HG3	2.16	0.45
1:B:369:GLU:OE1	1:B:391:ARG:HD2	2.16	0.45
1:B:199:GLY:O	1:B:200:SER:O	2.35	0.45
1:A:175:THR:HA	1:A:176:PRO:HD3	1.81	0.45
4:A:548:MPD:HM2	4:A:548:MPD:H4	1.74	0.44
1:B:62:LEU:HD22	1:B:173:ILE:HG22	1.98	0.44
1:B:215:ASP:O	1:B:219:ARG:HG3	2.17	0.44
1:A:66:LEU:O	1:A:70:LEU:HG	2.18	0.44
1:B:65:ASN:OD1	1:B:176:PRO:HG3	2.18	0.44
1:A:133:ARG:HB2	1:A:161:ASN:O	2.18	0.44
1:B:105:VAL:O	1:B:193:PHE:HB2	2.18	0.43
1:A:195:GLN:NE2	1:A:196:LEU:H	2.15	0.43
1:A:314:GLY:HA2	2:A:543:H90:C10	2.49	0.43
1:A:342:GLY:HA3	1:A:395:THR:HA	1.99	0.43
1:B:195:GLN:HE21	1:B:196:LEU:H	1.66	0.43
1:B:342:GLY:HA3	1:B:395:THR:HA	2.01	0.43
1:A:265:ASN:HB2	1:A:266:PRO:CD	2.49	0.43
1:B:371:LYS:HE2	1:B:415:TYR:CG	2.54	0.43
1:A:73:LYS:HG2	1:A:156:ILE:HD11	2.01	0.43
1:B:162:HIS:HB2	1:B:166:ASP:HB2	2.01	0.43
1:B:404:GLU:O	1:B:408:GLN:HG2	2.19	0.43
1:A:75:LEU:HD11	1:A:156:ILE:HD12	2.01	0.42
1:A:248:PRO:HD3	1:A:311:GLN:HE22	1.83	0.42
1:B:227:LEU:HD11	1:B:248:PRO:HB2	2.01	0.42
1:A:314:GLY:HA2	2:A:543:H90:C16	2.50	0.42
1:B:425:THR:HB	1:B:426:PRO:HD2	2.01	0.42
1:A:135:HIS:HE1	1:A:137:VAL:HG23	1.86	0.41
1:A:362:ARG:NE	6:A:578:HOH:O	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LYS:HE3	1:B:185:SER:O	2.20	0.41
1:A:27:ASP:HA	1:A:212:ASN:OD1	2.21	0.41
1:A:239:ALA:N	1:A:240:PRO:CD	2.83	0.41
1:A:267:GLU:HA	1:A:268:PRO:HD3	1.89	0.41
1:A:41:HIS:HB2	1:A:44:SER:OG	2.21	0.41
1:A:162:HIS:HB2	1:A:166:ASP:HB2	2.02	0.41
1:A:114:GLN:O	1:A:118:ASN:HB2	2.21	0.41
1:B:69:ARG:H	1:B:69:ARG:HG2	1.56	0.41
1:B:98:LEU:HD13	1:B:105:VAL:HB	2.02	0.41
1:B:27:ASP:HA	1:B:212:ASN:OD1	2.21	0.40
1:A:402:SER:N	1:A:403:PRO:HD3	2.36	0.40
1:A:118:ASN:HD22	1:A:143:PHE:HE1	1.67	0.40
1:A:305[A]:GLN:HE22	1:A:330:ASN:ND2	1.95	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	431/544 (79%)	420 (97%)	10 (2%)	1 (0%)	47	49
1	B	435/544 (80%)	422 (97%)	9 (2%)	4 (1%)	17	12
All	All	866/1088 (80%)	842 (97%)	19 (2%)	5 (1%)	25	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	SER
1	B	315	ALA
1	B	269	LEU
1	B	270	ASN
1	A	203	THR

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	366/472 (78%)	357 (98%)	9 (2%)	47	52
1	B	366/472 (78%)	357 (98%)	9 (2%)	47	52
All	All	732/944 (78%)	714 (98%)	18 (2%)	47	52

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	118	ASN
1	A	125	GLN
1	A	175	THR
1	A	195	GLN
1	A	213	ASP
1	A	223	GLU
1	A	228	ASN
1	A	396	PHE
1	B	44	SER
1	B	52	ARG
1	B	69	ARG
1	B	201	THR
1	B	213	ASP
1	B	295	GLU
1	B	391	ARG
1	B	396	PHE
1	B	433	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	21	ASN
1	A	118	ASN
1	A	195	GLN

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Mol	Chain	Res	Type
1	A	228	ASN
1	A	230	ASN
1	A	270	ASN
1	A	355	GLN
1	B	17	GLN
1	B	18	HIS
1	B	21	ASN
1	B	53	GLN
1	B	142	GLN
1	B	195	GLN
1	B	230	ASN
1	B	276	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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	MPD	A	548	-	7,7,7	0.35	0	9,10,10	0.59	0
5	MRD	B	547	-	7,7,7	0.33	0	9,10,10	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	H90	A	543	-	33,37,37	1.03	1 (3%)	41,52,52	1.84	6 (14%)
2	H90	B	543	-	33,37,37	0.97	2 (6%)	41,52,52	1.82	8 (19%)

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	MPD	A	548	-	-	0/5/5/5	-
5	MRD	B	547	-	-	2/5/5/5	-
2	H90	A	543	-	-	0/16/20/20	0/5/5/5
2	H90	B	543	-	-	0/16/20/20	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	543	H90	C16-C18	3.92	1.51	1.47
2	B	543	H90	C16-C18	3.26	1.50	1.47
2	B	543	H90	C10-C9	-2.14	1.37	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	543	H90	C11-C10-C9	6.14	110.88	105.20
2	B	543	H90	C11-C10-C9	5.81	110.57	105.20
2	A	543	H90	C3-C7-N8	-5.81	103.98	112.48
2	B	543	H90	C3-C7-N8	-4.65	105.67	112.48
2	B	543	H90	C16-C15-C14	-3.45	119.32	121.21
2	A	543	H90	C11-N12-N8	3.22	107.58	104.23
2	A	543	H90	C16-C15-C14	-3.06	119.54	121.21
2	A	543	H90	C18-C16-C10	-2.89	120.08	123.46
2	B	543	H90	C11-N12-N8	2.86	107.20	104.23
2	A	543	H90	C10-C11-N12	-2.83	104.55	110.43
2	B	543	H90	O27-C27-C24	-2.69	115.83	120.12
2	B	543	H90	C10-C11-N12	-2.67	104.90	110.43
2	B	543	H90	C28-C27-C24	2.23	123.95	120.28
2	B	543	H90	C26-C21-C22	2.21	121.99	117.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	547	MRD	C2-C3-C4-C5
5	B	547	MRD	C2-C3-C4-O4

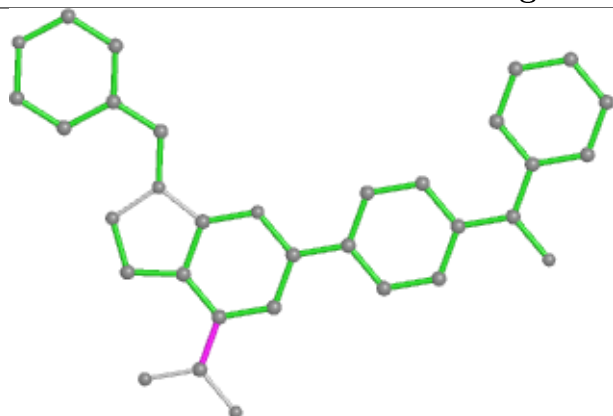
There are no ring outliers.

3 monomers are involved in 6 short contacts:

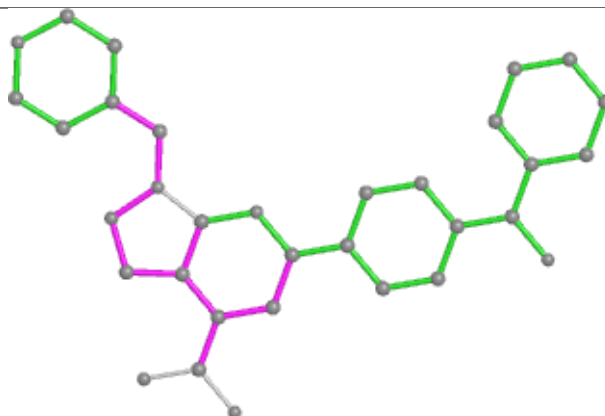
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	548	MPD	1	0
2	A	543	H90	3	0
2	B	543	H90	2	0

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 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.

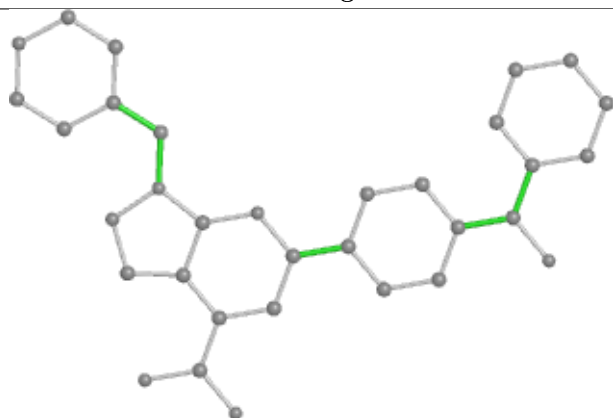
Ligand H90 A 543



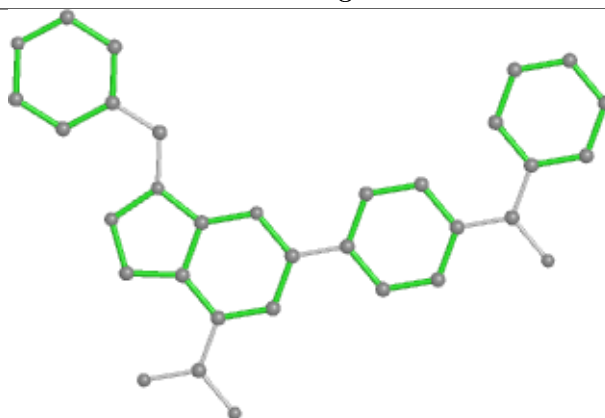
Bond lengths



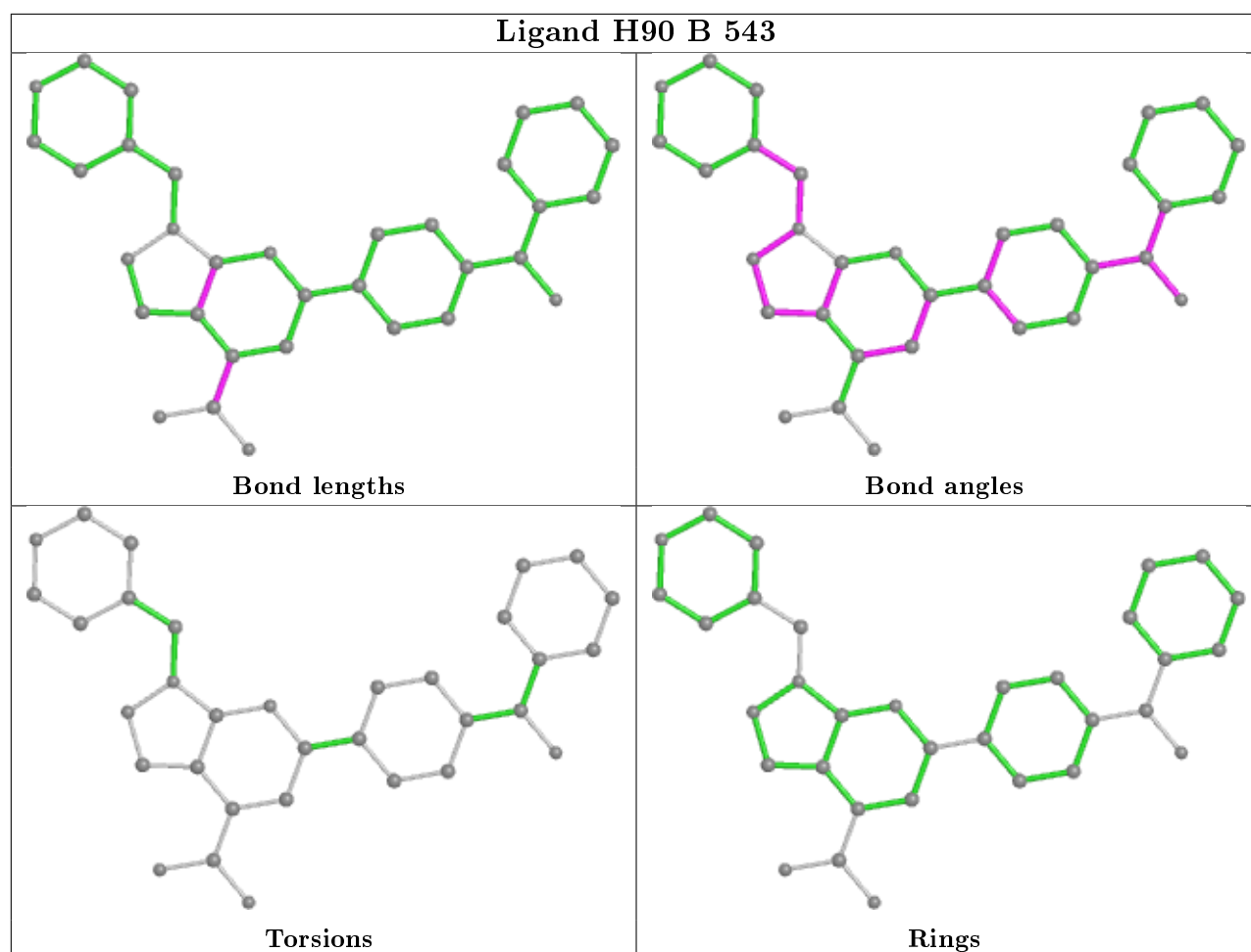
Bond angles



Torsions



Rings



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	433/544 (79%)	-0.03	16 (3%) 41 48	27, 37, 67, 84	0
1	B	436/544 (80%)	-0.16	10 (2%) 60 65	27, 39, 59, 76	0
All	All	869/1088 (79%)	-0.09	26 (2%) 50 56	27, 38, 64, 84	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	LEU	3.6
1	A	143	PHE	3.5
1	A	150	VAL	3.4
1	B	180	PHE	3.2
1	A	164	ALA	3.1
1	A	181	VAL	3.1
1	A	201	THR	2.9
1	A	179	THR	2.8
1	A	165	THR	2.7
1	B	148	HIS	2.7
1	A	426	PRO	2.7
1	A	167	PHE	2.6
1	B	149	ASP	2.5
1	B	150	VAL	2.4
1	A	376	GLN	2.4
1	A	177	ALA	2.3
1	B	201	THR	2.3
1	B	39	GLN	2.3
1	A	166	ASP	2.2
1	A	151	ASN	2.2
1	A	139	SER	2.2
1	B	382	GLU	2.1
1	B	179	THR	2.1
1	A	149	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	426	PRO	2.1
1	A	152	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

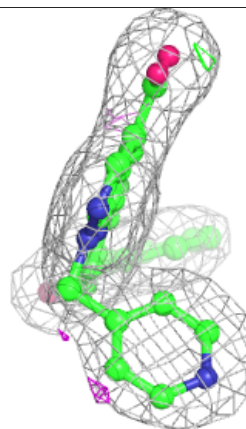
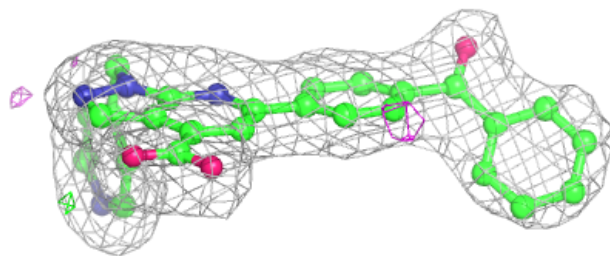
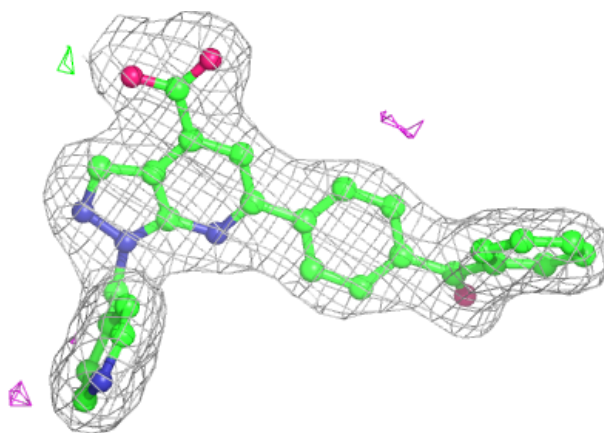
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	B	546	1/1	0.86	0.06	69,69,69,69	0
3	CA	A	547	1/1	0.88	0.16	73,73,73,73	0
3	CA	B	545	1/1	0.88	0.07	77,77,77,77	0
5	MRD	B	547	8/8	0.94	0.16	43,48,57,60	0
4	MPD	A	548	8/8	0.94	0.18	33,45,50,54	0
2	H90	A	543	33/33	0.96	0.14	22,33,46,48	0
3	CA	A	544	1/1	0.96	0.10	42,42,42,42	0
3	CA	B	544	1/1	0.97	0.10	48,48,48,48	0
2	H90	B	543	33/33	0.97	0.12	25,32,41,46	0
3	CA	A	546	1/1	0.98	0.10	35,35,35,35	0
3	CA	A	545	1/1	0.99	0.08	40,40,40,40	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.

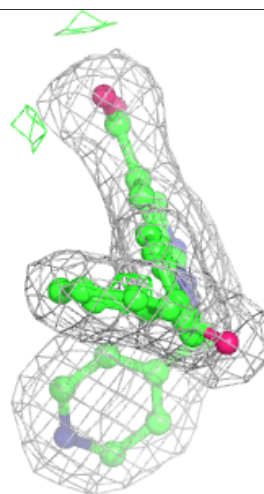
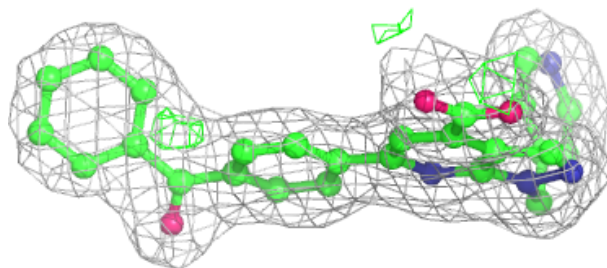
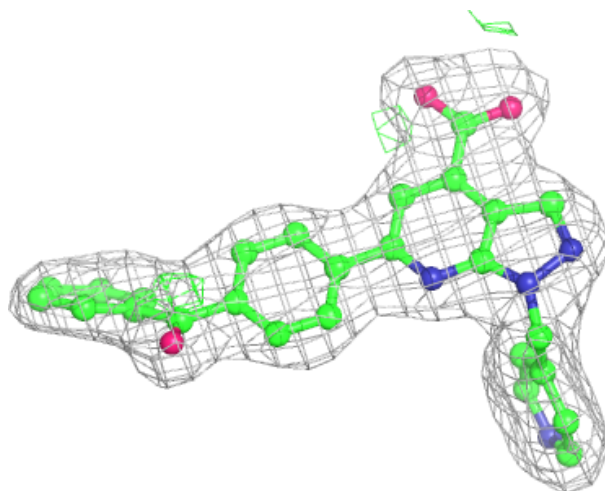
Electron density around H90 A 543:

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



Electron density around H90 B 543:

$2mF_o-DF_c$ (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.