



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:31 AM JST

PDB ID : 5YS0  
Title : Crystal structure of the second StARkin domain of Lam2 in complex with ergosterol  
Authors : Tong, J.; Im, Y.J.  
Deposited on : 2017-11-11  
Resolution : 2.60 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](mailto: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>.

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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 : 2.36  
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) : 2.36

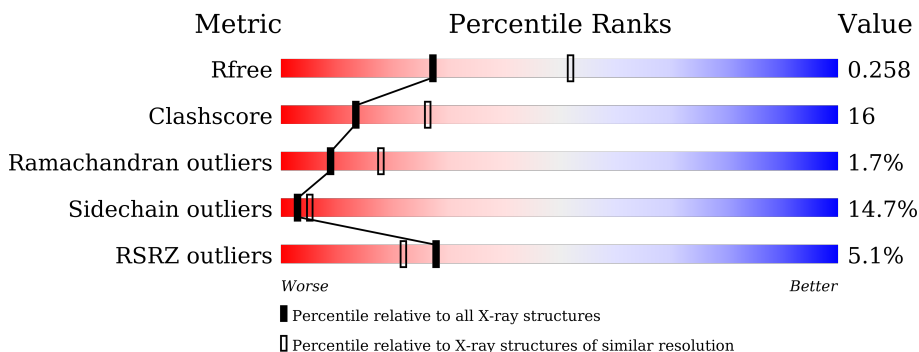
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	170	
1	B	170	
1	C	170	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ERG	A	1301	-	-	-	X
2	ERG	B	1301	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3854 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.

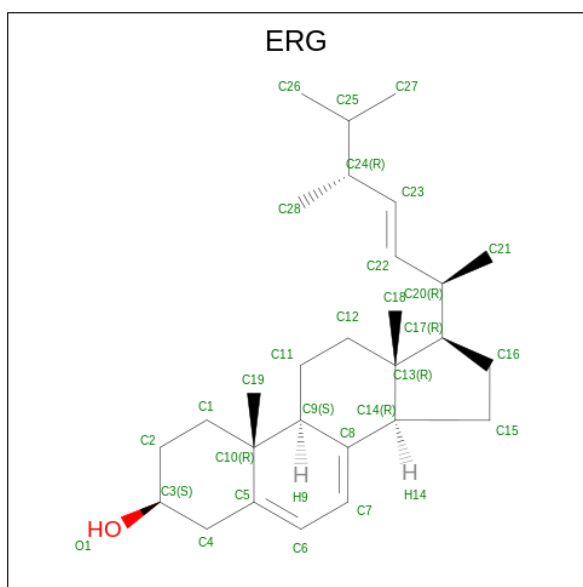
- Molecule 1 is a protein called Membrane-anchored lipid-binding protein YSP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	160	1279	816	214	243	6	0	0	0
1	B	164	1309	833	219	251	6	0	0	0
1	C	148	1187	760	196	225	6	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1054	GLY	-	expression tag	UNP Q06681
A	1055	SER	-	expression tag	UNP Q06681
A	1056	ALA	-	expression tag	UNP Q06681
A	1057	MET	-	expression tag	UNP Q06681
A	1058	GLY	-	expression tag	UNP Q06681
A	1059	SER	-	expression tag	UNP Q06681
B	1054	GLY	-	expression tag	UNP Q06681
B	1055	SER	-	expression tag	UNP Q06681
B	1056	ALA	-	expression tag	UNP Q06681
B	1057	MET	-	expression tag	UNP Q06681
B	1058	GLY	-	expression tag	UNP Q06681
B	1059	SER	-	expression tag	UNP Q06681
C	1054	GLY	-	expression tag	UNP Q06681
C	1055	SER	-	expression tag	UNP Q06681
C	1056	ALA	-	expression tag	UNP Q06681
C	1057	MET	-	expression tag	UNP Q06681
C	1058	GLY	-	expression tag	UNP Q06681
C	1059	SER	-	expression tag	UNP Q06681

- Molecule 2 is ERGOSTEROL (three-letter code: ERG) (formula: C<sub>28</sub>H<sub>44</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			29	28 1		
2	B	1	Total	C O	0	0
			29	28 1		

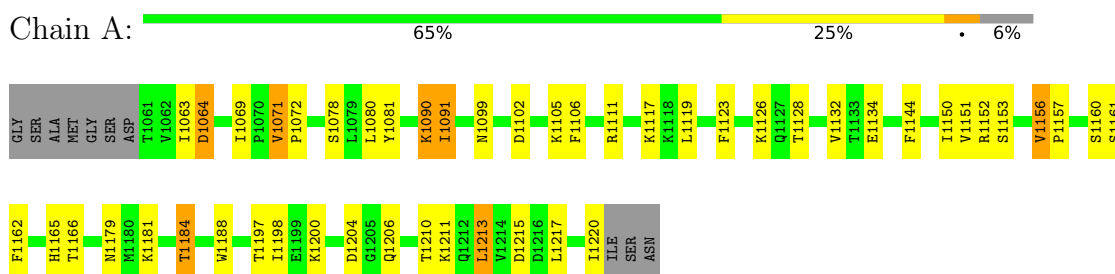
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	5	Total	O	0	0
			5	5		
3	C	6	Total	O	0	0
			6	6		

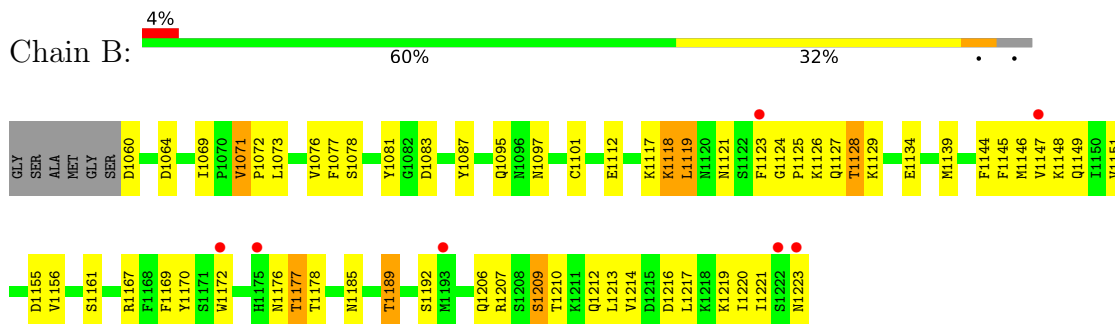
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

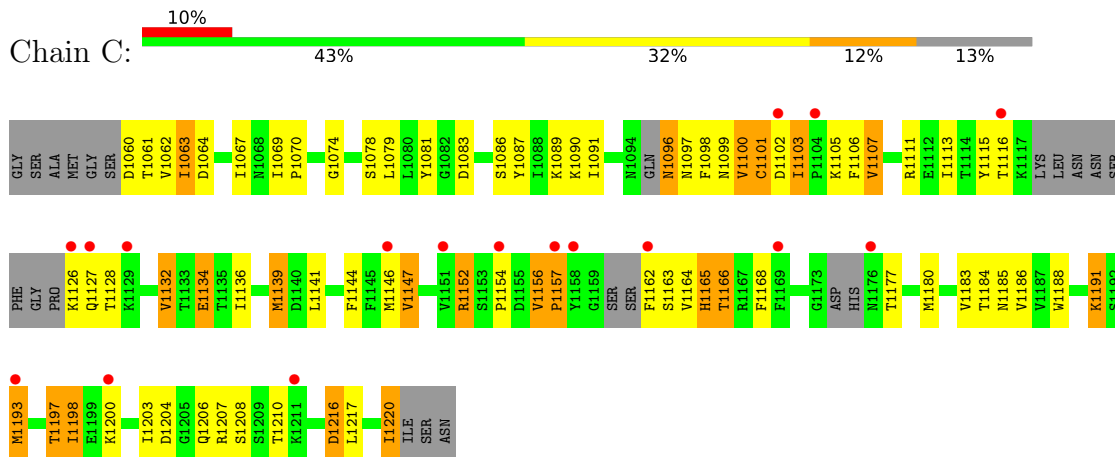
- Molecule 1: Membrane-anchored lipid-binding protein YSP2



- Molecule 1: Membrane-anchored lipid-binding protein YSP2



- Molecule 1: Membrane-anchored lipid-binding protein YSP2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.72Å 70.31Å 42.51Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	32.71 – 2.60 32.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (32.71-2.60) 98.9 (32.71-2.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.27 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.241 , 0.293 0.244 , 0.258	Depositor DCC
$R_{free}$ test set	830 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.026 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ERG

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	0.47	0/1305	0.63	0/1765
1	B	0.47	0/1335	0.62	0/1806
1	C	0.45	0/1206	0.60	0/1625
All	All	0.47	0/3846	0.62	0/5196

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	1279	0	1287	38	0
1	B	1309	0	1313	43	0
1	C	1187	0	1198	47	0
2	A	29	0	43	6	0
2	B	29	0	43	9	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
3	C	6	0	0	1	0
All	All	3854	0	3884	124	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 16.

All (124) 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:1087:TYR:HE2	1:C:1193:MET:HG3	1.39	0.88
1:A:1184:THR:HG21	1:A:1206:GLN:HG2	1.60	0.83
1:B:1076:VAL:HG21	1:B:1178:THR:HG21	1.61	0.81
1:C:1156:VAL:HB	1:C:1157:PRO:HD3	1.65	0.78
1:B:1087:TYR:CE2	1:C:1193:MET:HG3	2.22	0.75
1:B:1151:VAL:HG21	2:B:1301:ERG:H21	1.70	0.73
1:B:1069:ILE:HG13	1:B:1071:VAL:HG23	1.71	0.71
1:A:1117:LYS:HE3	2:A:1301:ERG:H191	1.73	0.70
1:A:1152:ARG:HH22	1:A:1160:SER:HA	1.55	0.70
1:A:1156:VAL:HG12	1:A:1157:PRO:HD2	1.74	0.69
1:A:1069:ILE:HG22	1:A:1071:VAL:HG23	1.76	0.67
1:A:1206:GLN:NE2	1:A:1210:THR:OG1	2.28	0.67
1:B:1125:PRO:HD2	2:B:1301:ERG:H283	1.77	0.67
1:C:1166:THR:HG23	1:C:1184:THR:HB	1.77	0.66
1:A:1091:ILE:HG21	1:A:1213:LEU:HD12	1.80	0.63
1:C:1105:LYS:O	1:C:1107:VAL:N	2.31	0.62
1:C:1067:ILE:HB	1:C:1180:MET:HB3	1.84	0.60
1:C:1204:ASP:HA	1:C:1207:ARG:HB3	1.84	0.59
1:B:1081:TYR:HH	1:B:1170:TYR:HH	1.51	0.59
1:B:1161:SER:HA	1:B:1189:THR:HG22	1.85	0.59
1:C:1146:MET:HG2	1:C:1168:PHE:O	2.03	0.59
1:A:1132:VAL:HG22	1:A:1151:VAL:HG22	1.85	0.58
1:B:1206:GLN:HA	1:B:1209:SER:HB2	1.86	0.58
1:B:1069:ILE:HD11	1:B:1076:VAL:HG22	1.86	0.57
1:C:1200:LYS:NZ	3:C:1301:HOH:O	2.38	0.57
1:B:1125:PRO:CD	2:B:1301:ERG:H283	2.33	0.56
1:C:1136:ILE:HG21	1:C:1139:MET:HG2	1.87	0.56
1:C:1096:ASN:HD22	1:C:1096:ASN:N	2.03	0.56
1:A:1090:LYS:HE2	3:A:1401:HOH:O	2.05	0.56
1:C:1188:TRP:CH2	1:C:1198:ILE:HG21	2.41	0.56
1:B:1151:VAL:HG21	2:B:1301:ERG:C2	2.36	0.56
1:A:1071:VAL:HG12	1:A:1072:PRO:HD2	1.87	0.55
1:C:1063:ILE:HG23	1:C:1207:ARG:HD2	1.89	0.55
1:B:1071:VAL:HG22	1:B:1221:ILE:HG13	1.88	0.55
1:C:1163:SER:HB2	1:C:1165:HIS:HE1	1.71	0.55
1:C:1101:CYS:SG	1:C:1102:ASP:N	2.80	0.54
1:A:1166:THR:HG23	1:A:1184:THR:HG22	1.88	0.54
1:A:1211:LYS:NZ	1:A:1215:ASP:OD2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1148:LYS:HE3	1:B:1167:ARG:CZ	2.38	0.54
1:C:1113:ILE:HG22	1:C:1115:TYR:CE2	2.42	0.54
1:B:1216:ASP:O	1:B:1220:ILE:HG13	2.08	0.53
1:A:1150:ILE:HG12	1:A:1165:HIS:CE1	2.44	0.53
1:A:1080:LEU:HD21	1:A:1217:LEU:HD13	1.91	0.52
1:B:1156:VAL:HG22	2:B:1301:ERG:H23	1.90	0.52
1:C:1206:GLN:O	1:C:1210:THR:HG23	2.11	0.51
1:B:1119:LEU:HD11	1:B:1128:THR:HG22	1.92	0.51
1:C:1113:ILE:HB	1:C:1132:VAL:HG12	1.92	0.51
1:C:1157:PRO:HG2	1:C:1198:ILE:HD11	1.92	0.51
1:A:1152:ARG:NH2	1:A:1162:PHE:O	2.44	0.50
1:C:1091:ILE:HD12	1:C:1216:ASP:HB3	1.92	0.50
1:C:1113:ILE:HG22	1:C:1115:TYR:HE2	1.75	0.50
1:B:1134:GLU:HG3	1:B:1149:GLN:HG3	1.94	0.50
1:A:1220:ILE:HD12	1:A:1220:ILE:H	1.77	0.49
1:B:1156:VAL:HG11	2:B:1301:ERG:H211	1.94	0.49
1:B:1119:LEU:HD21	2:B:1301:ERG:H181	1.94	0.49
1:C:1081:TYR:CZ	1:C:1147:VAL:HG21	2.48	0.49
1:B:1213:LEU:O	1:B:1217:LEU:HB2	2.12	0.49
1:C:1062:VAL:HG22	1:C:1183:VAL:HG12	1.95	0.49
1:B:1060:ASP:HA	1:B:1185:ASN:HB3	1.94	0.49
1:B:1206:GLN:O	1:B:1210:THR:HG23	2.13	0.48
1:C:1079:LEU:HD13	1:C:1220:ILE:HD12	1.96	0.48
1:C:1111:ARG:NE	1:C:1134:GLU:OE2	2.41	0.47
1:C:1141:LEU:HA	1:C:1141:LEU:HD23	1.52	0.47
1:A:1153:SER:O	1:A:1156:VAL:HG23	2.14	0.47
1:C:1111:ARG:HG3	1:C:1113:ILE:HD11	1.97	0.47
1:A:1081:TYR:HB3	1:A:1106:PHE:CE2	2.50	0.47
1:C:1197:THR:HG23	1:C:1200:LYS:HD2	1.97	0.47
1:B:1145:PHE:CE1	1:B:1170:TYR:HB2	2.50	0.46
1:A:1188:TRP:HH2	1:A:1198:ILE:HD12	1.81	0.46
1:C:1162:PHE:O	1:C:1162:PHE:CG	2.68	0.46
1:A:1102:ASP:OD1	1:B:1118:LYS:NZ	2.48	0.46
1:A:1119:LEU:HD11	1:A:1128:THR:HG22	1.97	0.46
1:B:1121:ASN:OD1	1:B:1123:PHE:HB2	2.16	0.46
1:C:1217:LEU:HD12	1:C:1217:LEU:HA	1.67	0.45
1:A:1151:VAL:HG21	2:A:1301:ERG:C2	2.47	0.45
1:C:1188:TRP:CZ2	1:C:1198:ILE:HG21	2.51	0.45
1:C:1074:GLY:HA2	1:C:1141:LEU:HD22	1.99	0.45
1:A:1162:PHE:HB3	1:A:1188:TRP:CE3	2.52	0.45
1:C:1163:SER:HB2	1:C:1165:HIS:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:ILE:O	1:B:1071:VAL:N	2.46	0.45
1:C:1089:LYS:HE2	1:C:1100:VAL:HB	1.98	0.45
1:A:1119:LEU:HB2	1:A:1126:LYS:HA	2.00	0.44
1:B:1117:LYS:O	1:B:1127:GLN:HA	2.17	0.44
1:C:1113:ILE:HB	1:C:1132:VAL:CG1	2.48	0.44
1:B:1071:VAL:CG2	1:B:1221:ILE:HG13	2.47	0.44
1:B:1071:VAL:HB	1:B:1076:VAL:HG23	2.00	0.44
1:B:1217:LEU:O	1:B:1221:ILE:HG12	2.18	0.44
1:C:1103:ILE:H	1:C:1103:ILE:HG12	1.58	0.44
1:C:1204:ASP:HA	1:C:1207:ARG:CB	2.47	0.43
1:B:1129:LYS:HG3	1:B:1155:ASP:OD2	2.18	0.43
1:A:1156:VAL:HG12	2:A:1301:ERG:H272	1.99	0.43
1:C:1191:LYS:HE3	1:C:1191:LYS:HB3	1.86	0.43
1:C:1152:ARG:HG2	1:C:1154:PRO:HD3	2.00	0.43
1:A:1069:ILE:O	1:A:1071:VAL:N	2.47	0.43
1:B:1071:VAL:HG12	1:B:1072:PRO:HD2	2.01	0.43
1:B:1210:THR:O	1:B:1214:VAL:HG13	2.18	0.43
1:B:1087:TYR:CD1	1:B:1087:TYR:N	2.86	0.43
1:A:1156:VAL:HG11	2:A:1301:ERG:H23	2.00	0.43
1:A:1213:LEU:O	1:A:1217:LEU:HB2	2.19	0.43
1:C:1087:TYR:OH	1:C:1220:ILE:HD13	2.18	0.43
1:A:1091:ILE:N	1:A:1091:ILE:HD13	2.33	0.43
1:C:1156:VAL:HB	1:C:1157:PRO:CD	2.40	0.42
1:B:1146:MET:HG3	1:B:1169:PHE:CE1	2.54	0.42
1:C:1188:TRP:HB2	1:C:1191:LYS:HG2	2.00	0.42
1:B:1156:VAL:HG21	2:B:1301:ERG:H20	2.00	0.42
1:A:1200:LYS:NZ	1:A:1200:LYS:HB3	2.35	0.42
1:A:1064:ASP:O	1:A:1181:LYS:HG3	2.20	0.42
1:C:1203:ILE:O	1:C:1207:ARG:HB2	2.20	0.42
1:A:1157:PRO:HG2	2:A:1301:ERG:H271	2.01	0.42
1:B:1177:THR:HG22	1:B:1178:THR:H	1.84	0.41
1:B:1124:GLY:HA3	2:B:1301:ERG:H281	2.02	0.41
1:A:1111:ARG:NE	1:A:1134:GLU:OE2	2.44	0.41
1:C:1126:LYS:HB2	1:C:1127:GLN:H	1.56	0.41
1:A:1211:LYS:O	1:A:1215:ASP:HB2	2.20	0.41
1:B:1081:TYR:CZ	1:B:1147:VAL:HG21	2.55	0.41
1:B:1077:PHE:HD1	1:B:1145:PHE:CE2	2.38	0.41
1:A:1151:VAL:HG11	2:A:1301:ERG:H193	2.03	0.41
1:A:1152:ARG:HH22	1:A:1160:SER:CA	2.28	0.41
1:C:1069:ILE:HA	1:C:1070:PRO:HD3	1.91	0.41
1:A:1099:ASN:OD1	1:B:1101:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1060:ASP:HA	1:C:1185:ASN:HB3	2.02	0.41
1:C:1164:VAL:HG22	1:C:1186:VAL:HG22	2.04	0.41
1:A:1063:ILE:CG1	1:A:1184:THR:HG23	2.52	0.40
1:B:1095:GLN:HB2	1:B:1097:ASN:ND2	2.36	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	158/170 (93%)	146 (92%)	12 (8%)	0	100	100
1	B	162/170 (95%)	143 (88%)	16 (10%)	3 (2%)	8	15
1	C	138/170 (81%)	115 (83%)	18 (13%)	5 (4%)	3	4
All	All	458/510 (90%)	404 (88%)	46 (10%)	8 (2%)	9	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1156	VAL
1	C	1063	ILE
1	C	1157	PRO
1	B	1073	LEU
1	C	1191	LYS
1	B	1172	TRP
1	C	1106	PHE
1	B	1176	ASN

### 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	150/157 (96%)	135 (90%)	15 (10%)	7	14
1	B	154/157 (98%)	135 (88%)	19 (12%)	4	9
1	C	139/157 (88%)	108 (78%)	31 (22%)	1	1
All	All	443/471 (94%)	378 (85%)	65 (15%)	3	5

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1064	ASP
1	A	1071	VAL
1	A	1078	SER
1	A	1090	LYS
1	A	1091	ILE
1	A	1105	LYS
1	A	1123	PHE
1	A	1144	PHE
1	A	1156	VAL
1	A	1161	SER
1	A	1179	ASN
1	A	1184	THR
1	A	1197	THR
1	A	1204	ASP
1	A	1213	LEU
1	B	1064	ASP
1	B	1071	VAL
1	B	1078	SER
1	B	1083	ASP
1	B	1112	GLU
1	B	1118	LYS
1	B	1119	LEU
1	B	1126	LYS
1	B	1128	THR
1	B	1139	MET
1	B	1144	PHE

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Mol	Chain	Res	Type
1	B	1177	THR
1	B	1189	THR
1	B	1192	SER
1	B	1207	ARG
1	B	1209	SER
1	B	1212	GLN
1	B	1219	LYS
1	B	1223	ASN
1	C	1061	THR
1	C	1064	ASP
1	C	1078	SER
1	C	1083	ASP
1	C	1086	SER
1	C	1090	LYS
1	C	1096	ASN
1	C	1097	ASN
1	C	1098	PHE
1	C	1099	ASN
1	C	1100	VAL
1	C	1101	CYS
1	C	1103	ILE
1	C	1107	VAL
1	C	1116	THR
1	C	1128	THR
1	C	1132	VAL
1	C	1134	GLU
1	C	1139	MET
1	C	1144	PHE
1	C	1147	VAL
1	C	1152	ARG
1	C	1165	HIS
1	C	1166	THR
1	C	1177	THR
1	C	1193	MET
1	C	1197	THR
1	C	1198	ILE
1	C	1208	SER
1	C	1216	ASP
1	C	1220	ILE

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	1121	ASN
1	A	1206	GLN
1	C	1165	HIS

### 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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ERG	B	1301	-	31,32,32	2.03	6 (19%)	47,50,50	1.66	9 (19%)
2	ERG	A	1301	-	31,32,32	2.05	6 (19%)	47,50,50	1.68	9 (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
2	ERG	B	1301	-	-	4/13/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ERG	A	1301	-	-	3/13/71/71	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ERG	C23-C22	7.07	1.53	1.32
2	B	1301	ERG	C23-C22	7.03	1.53	1.32
2	A	1301	ERG	C4-C5	-4.93	1.40	1.51
2	B	1301	ERG	C4-C5	-4.90	1.41	1.51
2	A	1301	ERG	C10-C5	-3.98	1.45	1.52
2	B	1301	ERG	C10-C5	-3.96	1.45	1.52
2	A	1301	ERG	C14-C8	-3.30	1.42	1.51
2	B	1301	ERG	C14-C8	-3.27	1.43	1.51
2	A	1301	ERG	C6-C5	3.16	1.41	1.33
2	B	1301	ERG	C6-C5	3.11	1.41	1.33
2	A	1301	ERG	C9-C8	-2.78	1.44	1.51
2	B	1301	ERG	C9-C8	-2.69	1.44	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	ERG	C4-C5-C10	4.54	122.45	116.42
2	B	1301	ERG	C4-C5-C10	4.50	122.40	116.42
2	A	1301	ERG	C14-C13-C17	-3.84	95.63	99.72
2	B	1301	ERG	C14-C13-C17	-3.81	95.67	99.72
2	A	1301	ERG	C18-C13-C14	3.52	115.96	110.24
2	B	1301	ERG	C18-C13-C14	3.51	115.93	110.24
2	A	1301	ERG	C16-C15-C14	-3.24	99.96	105.30
2	B	1301	ERG	C16-C15-C14	-3.23	99.98	105.30
2	A	1301	ERG	C24-C23-C22	-3.21	115.71	125.67
2	B	1301	ERG	C24-C23-C22	-3.18	115.79	125.67
2	A	1301	ERG	C20-C22-C23	-3.18	115.80	125.67
2	B	1301	ERG	C20-C22-C23	-3.15	115.88	125.67
2	A	1301	ERG	C14-C8-C9	2.85	118.94	114.66
2	B	1301	ERG	C14-C8-C9	2.75	118.79	114.66
2	A	1301	ERG	C14-C8-C7	-2.71	119.03	124.38
2	B	1301	ERG	C14-C8-C7	-2.62	119.22	124.38
2	A	1301	ERG	C15-C14-C13	-2.07	102.36	104.21
2	B	1301	ERG	C15-C14-C13	-2.04	102.39	104.21

There are no chirality outliers.



All (7) torsion outliers are listed below:

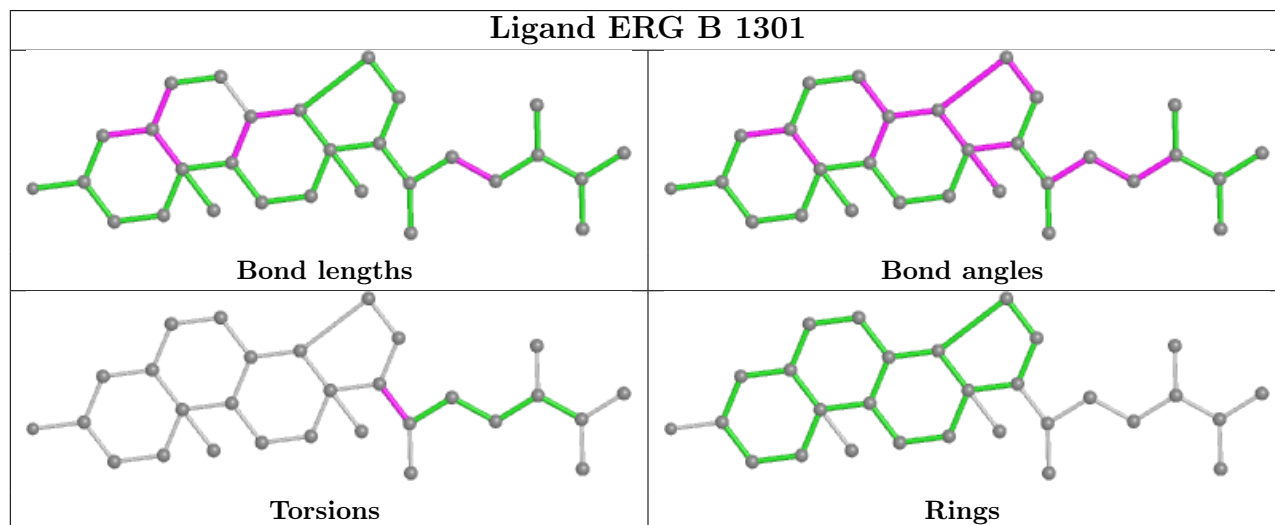
Mol	Chain	Res	Type	Atoms
2	B	1301	ERG	C16-C17-C20-C21
2	A	1301	ERG	C22-C23-C24-C25
2	B	1301	ERG	C13-C17-C20-C21
2	B	1301	ERG	C16-C17-C20-C22
2	A	1301	ERG	C17-C20-C22-C23
2	A	1301	ERG	C22-C23-C24-C28
2	B	1301	ERG	C13-C17-C20-C22

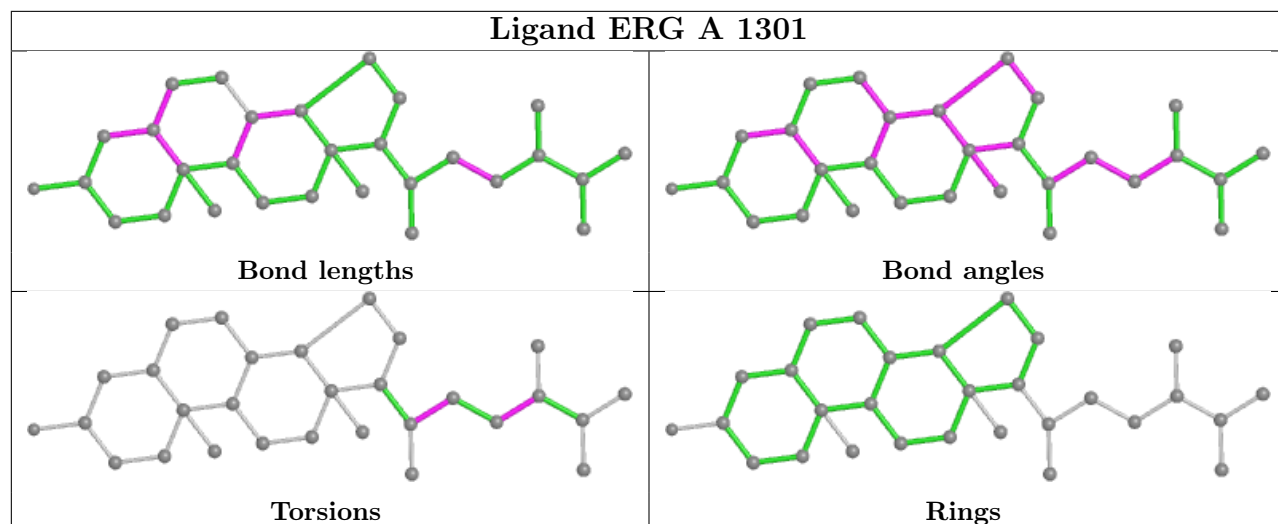
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	ERG	9	0
2	A	1301	ERG	6	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	160/170 (94%)	0.24	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	46, 66, 86, 104	0
1	B	164/170 (96%)	0.28	7 (4%) <span style="border: 1px solid red; padding: 2px;">35</span> <span style="border: 1px solid red; padding: 2px;">28</span>	45, 67, 94, 108	0
1	C	148/170 (87%)	0.73	17 (11%) <span style="border: 1px solid red; padding: 2px;">4</span> <span style="border: 1px solid red; padding: 2px;">3</span>	59, 89, 106, 124	0
All	All	472/510 (92%)	0.41	24 (5%) <span style="border: 1px solid red; padding: 2px;">28</span> <span style="border: 1px solid red; padding: 2px;">22</span>	45, 74, 100, 124	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1158	TYR	7.5
1	B	1222	SER	4.0
1	C	1126	LYS	2.8
1	C	1162	PHE	2.8
1	C	1193	MET	2.8
1	C	1129	LYS	2.7
1	C	1104	PRO	2.7
1	B	1123	PHE	2.6
1	B	1172	TRP	2.6
1	B	1175	HIS	2.5
1	C	1116	THR	2.5
1	C	1127	GLN	2.5
1	B	1223	ASN	2.3
1	C	1146	MET	2.2
1	C	1169	PHE	2.2
1	B	1147	VAL	2.1
1	C	1151	VAL	2.1
1	C	1102	ASP	2.1
1	C	1200	LYS	2.1
1	C	1176	ASN	2.1
1	B	1193	MET	2.0
1	C	1211	LYS	2.0
1	C	1154	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	1157	PRO	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](#)

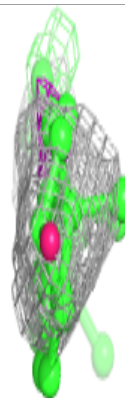
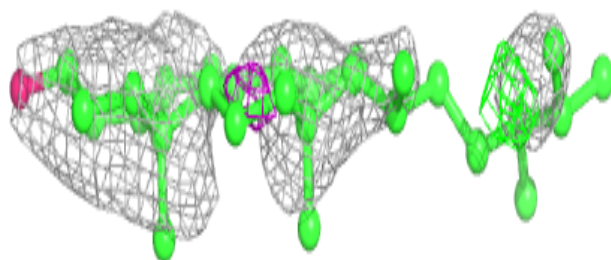
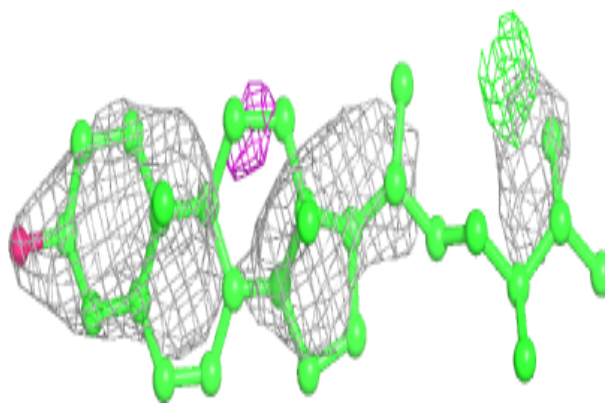
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ERG	B	1301	29/29	0.74	0.45	65,74,83,86	29
2	ERG	A	1301	29/29	0.77	0.42	65,76,86,89	29

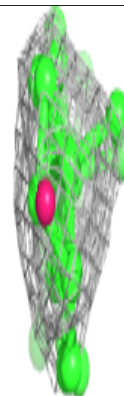
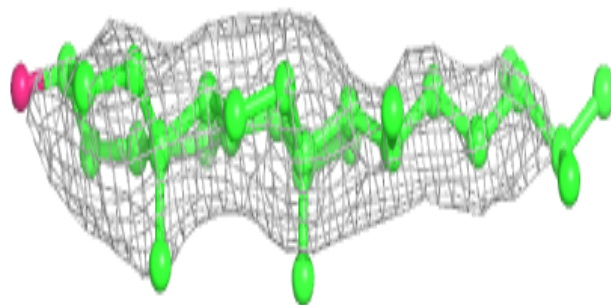
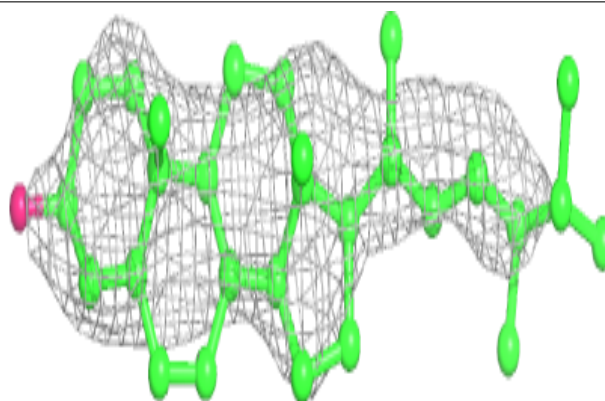
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ERG 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)

**Electron density around ERG A 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.