



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 7L0O / pdb_00007l0o
Title : Streptococcus gordonii C123 Domain(s)-Structural and Functional Analysis
Authors : Schormann, N.; Deivanayagam, C.
Deposited on : 2020-12-11
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

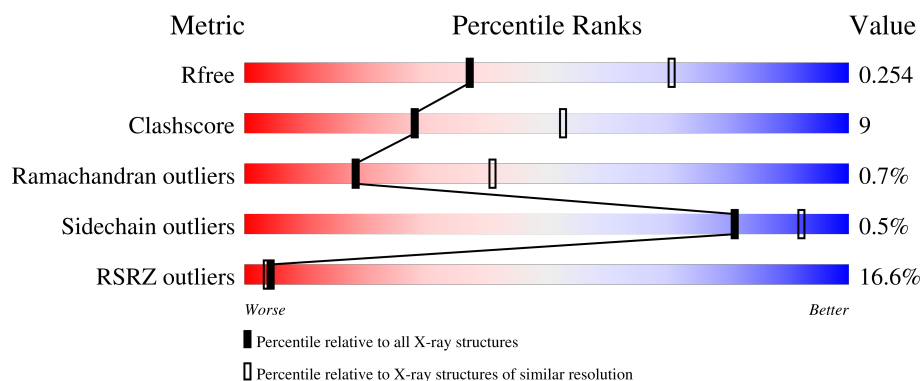
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	507	15% 74% 20% 6%
1	B	507	16% 76% 18% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7511 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 Agglutinin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3745	2365	608	769	3			
1	B	476	Total	C	N	O	S	0	0	0
			3721	2351	602	765	3			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	911	MET	-	initiating methionine	UNP P16952
A	912	ALA	-	expression tag	UNP P16952
A	1407	ALA	-	expression tag	UNP P16952
A	1408	ALA	-	expression tag	UNP P16952
A	1409	ALA	-	expression tag	UNP P16952
A	1410	LEU	-	expression tag	UNP P16952
A	1411	GLU	-	expression tag	UNP P16952
A	1412	HIS	-	expression tag	UNP P16952
A	1413	HIS	-	expression tag	UNP P16952
A	1414	HIS	-	expression tag	UNP P16952
A	1415	HIS	-	expression tag	UNP P16952
A	1416	HIS	-	expression tag	UNP P16952
A	1417	HIS	-	expression tag	UNP P16952
B	911	MET	-	initiating methionine	UNP P16952
B	912	ALA	-	expression tag	UNP P16952
B	1407	ALA	-	expression tag	UNP P16952
B	1408	ALA	-	expression tag	UNP P16952
B	1409	ALA	-	expression tag	UNP P16952
B	1410	LEU	-	expression tag	UNP P16952
B	1411	GLU	-	expression tag	UNP P16952
B	1412	HIS	-	expression tag	UNP P16952
B	1413	HIS	-	expression tag	UNP P16952
B	1414	HIS	-	expression tag	UNP P16952
B	1415	HIS	-	expression tag	UNP P16952
B	1416	HIS	-	expression tag	UNP P16952

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1417	HIS	-	expression tag	UNP P16952

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

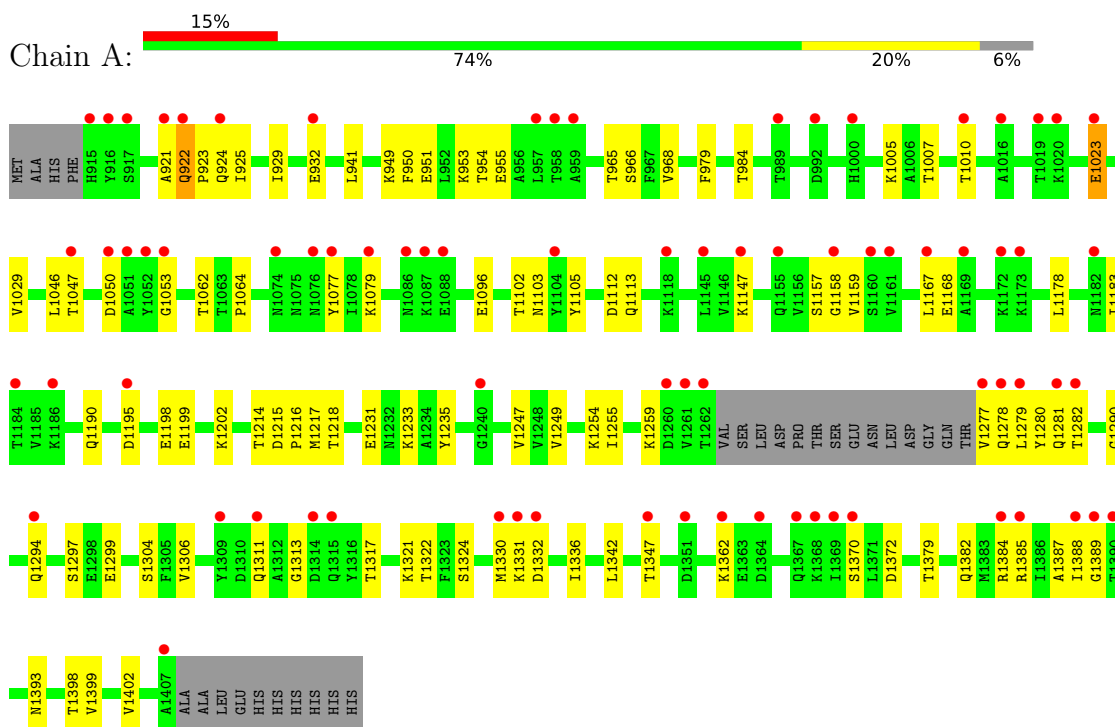
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	21	Total O 21 21	0	0
3	B	20	Total O 20 20	0	0

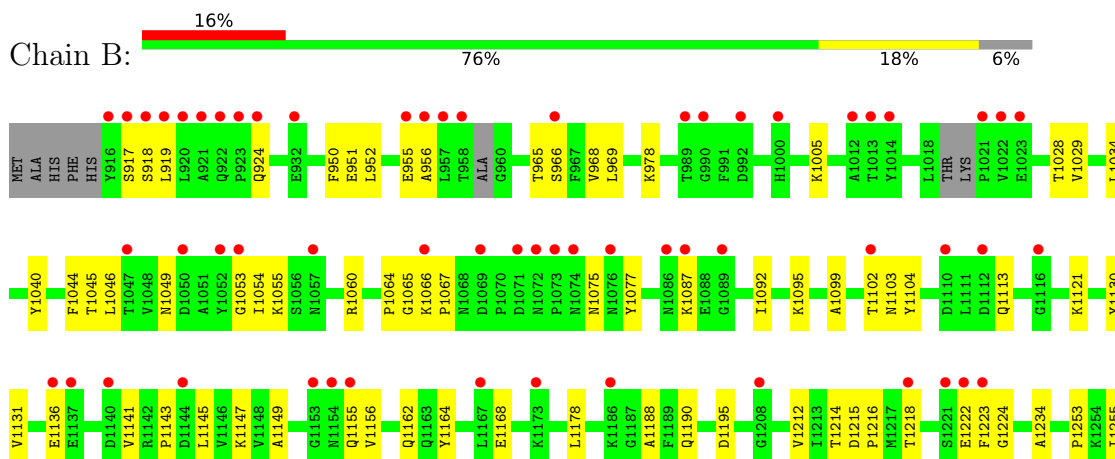
3 Residue-property plots

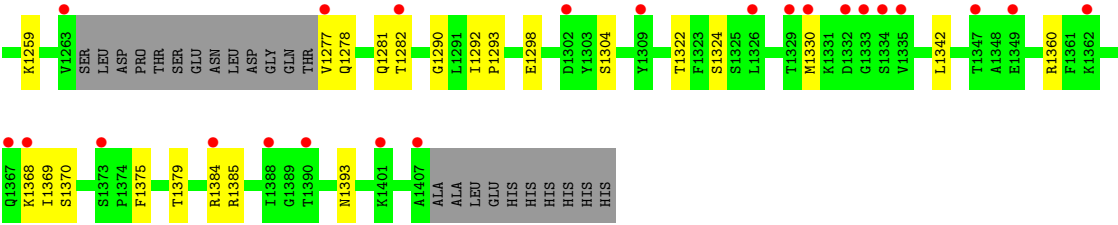
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Agglutinin receptor



• Molecule 1: Agglutinin receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.05Å 109.14Å 204.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.70 48.59 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (48.59-2.70) 96.7 (48.59-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
R, R_{free}	0.218 , 0.255 0.220 , 0.254	Depositor DCC
R_{free} test set	2854 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.923	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7511	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: CA

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	0.31	0/3816	0.54	2/5187 (0.0%)
1	B	0.26	0/3789	0.48	0/5147
All	All	0.29	0/7605	0.51	2/10334 (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	922	GLN	CA-C-N	-5.94	114.11	120.47
1	A	922	GLN	C-N-CA	-5.94	114.11	120.47

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	3745	0	3646	73	0
1	B	3721	0	3621	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	21	0	0	2	0
3	B	20	0	0	0	0
All	All	7511	0	7267	131	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 (131) 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:922:GLN:CG	1:A:923:PRO:HD3	1.63	1.28
1:A:922:GLN:HG2	1:A:923:PRO:CD	1.63	1.25
1:A:1306:VAL:HG21	1:B:1222:GLU:OE1	1.76	0.86
1:A:923:PRO:HD2	1:A:955:GLU:HG3	1.58	0.83
1:A:1112:ASP:OD1	1:A:1113:GLN:N	2.14	0.80
1:B:1102:THR:HG23	1:B:1218:THR:HG22	1.63	0.80
1:B:1066:LYS:HD2	1:B:1067:PRO:HD2	1.65	0.79
1:A:1282:THR:HG22	1:A:1384:ARG:HD2	1.68	0.76
1:A:1023:GLU:H	1:A:1023:GLU:CD	1.94	0.75
1:B:1190:GLN:NE2	1:B:1215:ASP:OD2	2.20	0.74
1:B:1322:THR:HG22	1:B:1379:THR:HG22	1.69	0.73
1:A:1304:SER:OG	1:A:1398:THR:HB	1.87	0.73
1:A:1259:LYS:NZ	1:A:1393:ASN:O	2.25	0.69
1:A:1277:VAL:HG13	1:A:1278:GLN:H	1.56	0.69
1:A:941:LEU:HD11	1:A:1064:PRO:N	2.08	0.68
1:A:1279:LEU:HG	1:A:1280:TYR:CD2	2.29	0.67
1:A:941:LEU:HD12	1:A:1062:THR:O	1.95	0.67
1:B:1045:THR:HG22	1:B:1055:LYS:HD2	1.79	0.65
1:A:941:LEU:HD11	1:A:1064:PRO:CD	2.27	0.64
1:A:968:VAL:HG22	1:A:1005:LYS:HG2	1.78	0.64
1:A:1231:GLU:HG2	1:A:1249:VAL:HG22	1.79	0.64
1:A:1198:GLU:HG3	1:A:1202:LYS:HE3	1.79	0.64
1:A:1190:GLN:NE2	1:A:1215:ASP:OD2	2.29	0.64
1:B:1304:SER:HB2	1:B:1360:ARG:HG2	1.80	0.63
1:B:1255:ILE:HG23	1:B:1290:GLY:HA3	1.81	0.63
1:A:1077:TYR:HB2	1:A:1079:LYS:NZ	2.15	0.62
1:A:941:LEU:HD11	1:A:1064:PRO:HD3	1.81	0.61
1:B:1330:MET:HB2	1:B:1368:LYS:O	2.02	0.59
1:A:1277:VAL:HG13	1:A:1278:GLN:N	2.16	0.59
1:B:1147:LYS:HG2	1:B:1214:THR:OG1	2.02	0.59
1:A:1294:GLN:HG3	1:A:1372:ASP:O	2.03	0.59
1:A:1385:ARG:NH1	1:A:1389:GLY:O	2.36	0.59
1:A:1347:THR:OG1	1:A:1362:LYS:NZ	2.31	0.58
1:A:1233:LYS:HD3	1:A:1247:VAL:HG22	1.86	0.58
1:A:1330:MET:HG3	1:A:1332:ASP:OD1	2.04	0.58
1:B:965:THR:HG23	1:B:1049:ASN:HA	1.86	0.57
1:B:918:SER:OG	1:B:919:LEU:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:GLU:N	1:A:1023:GLU:OE2	2.36	0.56
1:B:950:PHE:HB2	1:B:1029:VAL:HB	1.86	0.56
1:A:1254:LYS:HA	3:A:1602:HOH:O	2.04	0.56
1:A:1330:MET:HA	1:A:1370:SER:H	1.71	0.56
1:B:1099:ALA:HB2	1:B:1224:GLY:HA3	1.88	0.55
1:A:1399:VAL:O	1:A:1402:VAL:HG12	2.07	0.54
1:B:1298:GLU:OE1	1:B:1298:GLU:N	2.34	0.54
1:A:1282:THR:HG22	1:A:1384:ARG:CD	2.35	0.54
1:A:1096:GLU:O	1:A:1297:SER:OG	2.22	0.54
1:A:1147:LYS:HG2	1:A:1214:THR:OG1	2.08	0.54
1:B:1064:PRO:HA	1:B:1075:ASN:HD21	1.71	0.54
1:A:1077:TYR:HB2	1:A:1079:LYS:HZ3	1.72	0.53
1:A:950:PHE:HB2	1:A:1029:VAL:HB	1.90	0.53
1:A:1324:SER:HB3	1:A:1342:LEU:HD11	1.89	0.53
1:A:1282:THR:HG22	1:A:1384:ARG:CG	2.40	0.52
1:B:1259:LYS:NZ	1:B:1393:ASN:O	2.38	0.52
1:B:969:LEU:HD23	1:B:1046:LEU:HB2	1.90	0.52
1:A:1277:VAL:CG1	1:A:1278:GLN:H	2.22	0.51
1:B:1064:PRO:HA	1:B:1075:ASN:ND2	2.26	0.50
1:B:1324:SER:HB3	1:B:1342:LEU:HD11	1.93	0.50
1:B:1075:ASN:ND2	1:B:1113:GLN:HB2	2.26	0.50
1:A:1007:THR:OG1	1:A:1010:THR:HG22	2.11	0.49
1:B:1092:ILE:HG22	1:B:1095:LYS:HD2	1.94	0.49
1:A:922:GLN:HG2	1:A:923:PRO:HD3	0.71	0.49
1:B:1065:GLY:H	1:B:1075:ASN:HD21	1.60	0.49
1:A:1299:GLU:OE2	1:A:1331:LYS:NZ	2.38	0.49
1:B:1147:LYS:CG	1:B:1214:THR:OG1	2.60	0.48
1:A:1255:ILE:HG23	1:A:1290:GLY:HA3	1.95	0.48
1:A:922:GLN:CD	1:A:923:PRO:HD3	2.35	0.48
1:B:1103:ASN:O	1:B:1216:PRO:HA	2.14	0.48
1:A:932:GLU:HA	1:A:949:LYS:NZ	2.29	0.47
1:A:965:THR:OG1	1:A:966:SER:N	2.47	0.47
1:A:1077:TYR:HB2	1:A:1079:LYS:CE	2.44	0.47
1:A:1157:SER:O	1:A:1159:VAL:N	2.42	0.47
1:A:1103:ASN:O	1:A:1216:PRO:HA	2.14	0.47
1:B:917:SER:O	1:B:918:SER:HB3	2.13	0.47
1:A:925:ILE:HG22	1:A:954:THR:HG22	1.96	0.47
1:A:1047:THR:HA	1:A:1053:GLY:HA2	1.97	0.47
1:A:1167:LEU:HD13	1:A:1178:LEU:HD12	1.97	0.47
1:A:1322:THR:HG22	1:A:1379:THR:HG22	1.97	0.47
1:B:965:THR:HG23	1:B:966:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1277:VAL:HA	1:B:1385:ARG:NH1	2.29	0.47
1:A:1311:GLN:H	1:A:1311:GLN:CD	2.23	0.46
1:A:951:GLU:OE2	1:A:953:LYS:HE2	2.15	0.46
1:B:965:THR:CG2	1:B:1049:ASN:HA	2.45	0.46
1:B:924:GLN:O	1:B:955:GLU:HG3	2.15	0.46
1:A:941:LEU:CD1	1:A:1064:PRO:HD3	2.45	0.46
1:A:1330:MET:HE1	1:A:1336:ILE:HG13	1.96	0.46
1:A:1147:LYS:CG	1:A:1214:THR:OG1	2.64	0.45
1:B:1253:PRO:HB3	1:B:1293:PRO:HG3	1.98	0.45
1:B:1067:PRO:HG3	1:B:1077:TYR:HE1	1.81	0.45
1:B:1053:GLY:O	1:B:1054:ILE:HD13	2.17	0.45
1:A:1046:LEU:O	1:A:1053:GLY:HA2	2.16	0.45
1:A:1168:GLU:H	1:A:1168:GLU:CD	2.25	0.45
1:B:1121:LYS:HD3	1:B:1121:LYS:HA	1.71	0.45
1:A:1313:GLY:HA2	1:A:1387:ALA:HB3	1.99	0.45
1:B:978:LYS:HB2	1:B:1034:LEU:HD11	1.98	0.44
1:B:1087:LYS:HG3	1:B:1104:TYR:CZ	2.52	0.44
1:A:1317:THR:HG21	1:A:1382:GLN:HG2	1.99	0.44
1:B:952:LEU:HD22	1:B:1044:PHE:CD1	2.53	0.44
1:A:932:GLU:HA	1:A:949:LYS:HZ2	1.83	0.44
1:A:1183:ILE:HD12	1:A:1235:TYR:CD2	2.52	0.44
1:B:1330:MET:HB2	1:B:1369:ILE:HA	1.99	0.44
1:B:951:GLU:HG2	1:B:1028:THR:HG22	2.00	0.43
1:B:1075:ASN:HD22	1:B:1113:GLN:HB2	1.81	0.43
1:A:929:ILE:HD12	1:A:950:PHE:HE1	1.83	0.43
1:B:1130:TYR:HE1	1:B:1234:ALA:HB1	1.83	0.43
1:B:1155:GLN:HG2	1:B:1156:VAL:N	2.34	0.43
1:A:979:PHE:CE2	1:A:984:THR:HG21	2.53	0.43
1:A:1105:TYR:HD2	1:A:1217:MET:HE3	1.83	0.43
1:A:1277:VAL:O	1:A:1281:GLN:HB3	2.19	0.43
1:B:1168:GLU:N	1:B:1168:GLU:OE1	2.52	0.43
1:B:1141:VAL:O	1:B:1143:PRO:HD3	2.19	0.43
1:B:1282:THR:HG22	1:B:1384:ARG:HG2	2.00	0.43
1:B:1149:ALA:O	1:B:1212:VAL:N	2.38	0.43
1:B:1040:TYR:O	1:B:1060:ARG:HA	2.19	0.43
1:A:1102:THR:OG1	1:A:1218:THR:HG22	2.19	0.42
1:A:1023:GLU:CD	1:A:1023:GLU:N	2.72	0.42
1:B:1136:GLU:HB3	1:B:1188:ALA:HB3	2.01	0.42
1:A:1385:ARG:HG2	1:A:1387:ALA:O	2.20	0.42
1:B:1145:LEU:HB3	1:B:1216:PRO:HG2	2.02	0.42
1:B:1131:VAL:HG21	1:B:1178:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1162:GLN:HG2	1:B:1164:TYR:CZ	2.55	0.41
1:B:1155:GLN:HG2	1:B:1156:VAL:H	1.85	0.41
1:A:1388:ILE:HD12	1:A:1388:ILE:HA	1.96	0.41
1:B:969:LEU:HD22	1:B:1044:PHE:CE2	2.55	0.41
1:B:968:VAL:HG22	1:B:1005:LYS:HG2	2.01	0.41
1:B:1278:GLN:O	1:B:1281:GLN:HB3	2.21	0.41
1:A:1277:VAL:CG1	1:A:1278:GLN:N	2.82	0.41
1:B:1099:ALA:HB2	1:B:1224:GLY:CA	2.51	0.41
1:B:1292:ILE:HB	1:B:1375:PHE:HB3	2.02	0.41
1:B:1330:MET:HA	1:B:1370:SER:H	1.87	0.41
1:A:1112:ASP:OD1	3:A:1601:HOH:O	2.22	0.40
1:B:1277:VAL:N	1:B:1281:GLN:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	475/507 (94%)	446 (94%)	24 (5%)	5 (1%)	11	29
1	B	468/507 (92%)	438 (94%)	28 (6%)	2 (0%)	30	54
All	All	943/1014 (93%)	884 (94%)	52 (6%)	7 (1%)	18	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	921	ALA
1	A	1158	GLY
1	B	956	ALA
1	B	1195	ASP
1	A	924	GLN
1	A	1195	ASP

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Mol	Chain	Res	Type
1	A	1050	ASP

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	415/439 (94%)	412 (99%)	3 (1%)	76	90
1	B	413/439 (94%)	412 (100%)	1 (0%)	87	95
All	All	828/878 (94%)	824 (100%)	4 (0%)	81	92

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

Mol	Chain	Res	Type
1	A	1023	GLU
1	A	1199	GLU
1	A	1321	LYS
1	B	1223	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1068	ASN
1	A	1154	ASN
1	A	1284	ASN
1	B	1075	ASN
1	B	1162	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	479/507 (94%)	0.99	77 (16%) 4 4	54, 86, 128, 157	0
1	B	476/507 (93%)	1.11	82 (17%) 4 3	54, 86, 130, 154	0
All	All	955/1014 (94%)	1.05	159 (16%) 4 4	54, 86, 128, 157	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	919	LEU	6.3
1	B	958	THR	5.7
1	B	1407	ALA	5.6
1	B	1022	VAL	5.4
1	B	1050	ASP	5.4
1	A	1050	ASP	5.2
1	A	1362	LYS	5.2
1	B	918	SER	5.2
1	B	956	ALA	5.1
1	A	1158	GLY	5.1
1	B	1013	THR	4.8
1	B	1021	PRO	4.7
1	B	989	THR	4.7
1	B	923	PRO	4.6
1	B	1277	VAL	4.5
1	B	1221	SER	4.5
1	B	1047	THR	4.5
1	B	1052	TYR	4.4
1	A	916	TYR	4.3
1	B	921	ALA	4.3
1	A	1407	ALA	4.2
1	A	1330	MET	4.2
1	A	1010	THR	4.1
1	A	1172	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1370	SER	4.0
1	B	920	LEU	4.0
1	A	915	HIS	3.9
1	A	1277	VAL	3.8
1	A	1384	ARG	3.8
1	B	1330	MET	3.7
1	A	1281	GLN	3.7
1	B	1362	LYS	3.7
1	B	932	GLU	3.6
1	B	917	SER	3.5
1	A	1079	LYS	3.4
1	A	1155	GLN	3.4
1	B	955	GLU	3.4
1	B	1072	ASN	3.4
1	A	959	ALA	3.4
1	A	1279	LEU	3.4
1	A	1023	GLU	3.3
1	A	1088	GLU	3.3
1	A	1173	LYS	3.3
1	A	1086	ASN	3.3
1	B	1110	ASP	3.3
1	B	1333	GLY	3.3
1	A	1169	ALA	3.3
1	B	1112	ASP	3.2
1	A	1368	LYS	3.2
1	B	1218	THR	3.2
1	B	1023	GLU	3.1
1	B	922	GLN	3.1
1	B	1155	GLN	3.1
1	A	1282	THR	3.1
1	A	921	ALA	3.0
1	B	1309	TYR	3.0
1	A	1347	THR	3.0
1	A	922	GLN	2.9
1	B	1208	GLY	2.9
1	A	1262	THR	2.9
1	A	1000	HIS	2.9
1	A	1182	ASN	2.9
1	B	1347	THR	2.9
1	B	1076	ASN	2.9
1	B	1329	THR	2.9
1	A	1104	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1326	LEU	2.9
1	B	1074	ASN	2.8
1	A	1053	GLY	2.8
1	B	1154	ASN	2.8
1	A	1186	LYS	2.8
1	B	924	GLN	2.8
1	B	1367	GLN	2.8
1	A	1332	ASP	2.8
1	B	1390	THR	2.8
1	A	917	SER	2.7
1	A	1278	GLN	2.7
1	B	1167	LEU	2.7
1	A	932	GLU	2.7
1	A	1385	ARG	2.7
1	B	1332	ASP	2.7
1	A	1331	LYS	2.7
1	A	1167	LEU	2.7
1	B	1153	GLY	2.7
1	B	1087	LYS	2.7
1	A	1087	LYS	2.6
1	A	1077	TYR	2.6
1	B	1173	LYS	2.6
1	A	1051	ALA	2.6
1	B	1102	THR	2.5
1	A	1389	GLY	2.5
1	A	1309	TYR	2.5
1	B	1222	GLU	2.5
1	A	1364	ASP	2.5
1	B	1066	LYS	2.5
1	B	1349	GLU	2.5
1	A	1161	VAL	2.5
1	B	1335	VAL	2.5
1	A	1351	ASP	2.5
1	B	1071	ASP	2.5
1	B	916	TYR	2.5
1	A	1019	THR	2.4
1	B	990	GLY	2.4
1	A	1074	ASN	2.4
1	A	1076	ASN	2.4
1	B	1137	GLU	2.4
1	A	1314	ASP	2.4
1	A	1118	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	958	THR	2.3
1	B	1086	ASN	2.3
1	A	1160	SER	2.3
1	A	1184	THR	2.3
1	A	957	LEU	2.3
1	B	957	LEU	2.3
1	B	1057	ASN	2.3
1	A	1315	GLN	2.3
1	A	1261	VAL	2.3
1	B	1282	THR	2.3
1	B	1053	GLY	2.3
1	A	1145	LEU	2.3
1	A	1147	LYS	2.2
1	A	1052	TYR	2.2
1	A	1311	GLN	2.2
1	B	1089	GLY	2.2
1	A	1388	ILE	2.2
1	B	1116	GLY	2.2
1	A	1369	ILE	2.2
1	B	1388	ILE	2.2
1	B	1136	GLU	2.2
1	B	1384	ARG	2.2
1	B	992	ASP	2.2
1	B	1373	SER	2.2
1	B	1012	ALA	2.2
1	B	1014	TYR	2.2
1	A	1020	LYS	2.2
1	B	1186	LYS	2.2
1	B	1069	ASP	2.2
1	B	1334	SER	2.2
1	B	1223	PHE	2.2
1	A	992	ASP	2.1
1	A	1047	THR	2.1
1	A	1390	THR	2.1
1	B	1073	PRO	2.1
1	A	1367	GLN	2.1
1	B	1144	ASP	2.1
1	B	1368	LYS	2.1
1	A	924	GLN	2.1
1	A	1294	GLN	2.1
1	B	1000	HIS	2.1
1	A	1195	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1260	ASP	2.0
1	B	1140	ASP	2.0
1	A	989	THR	2.0
1	A	1240	GLY	2.0
1	A	1016	ALA	2.0
1	B	1302	ASP	2.0
1	B	1401	LYS	2.0
1	B	966	SER	2.0
1	B	1263	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

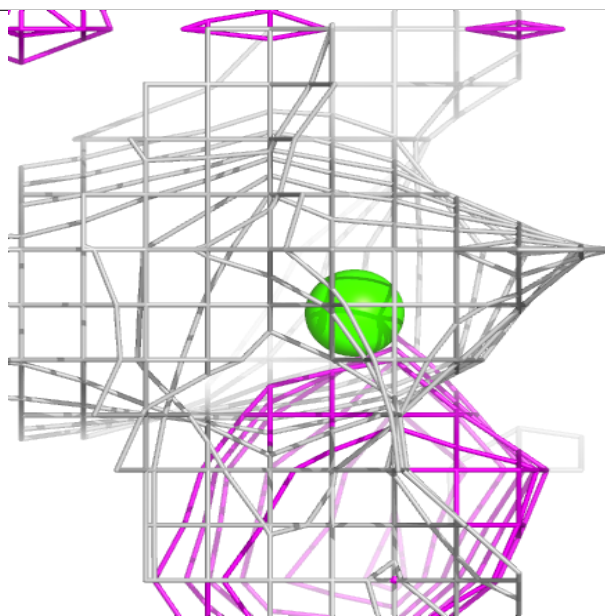
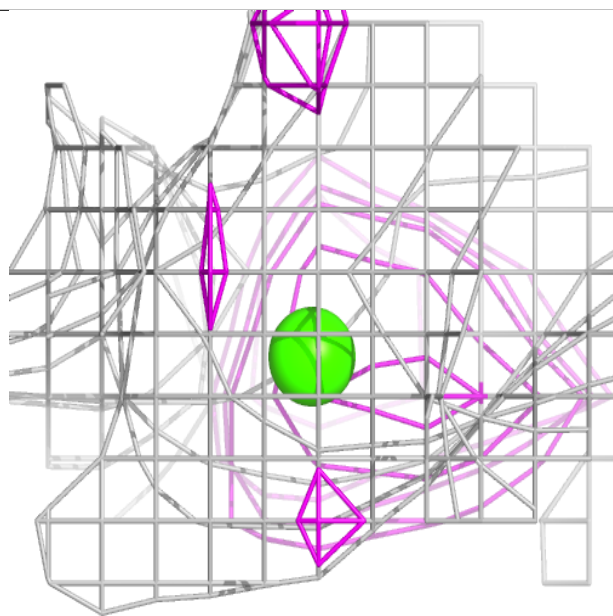
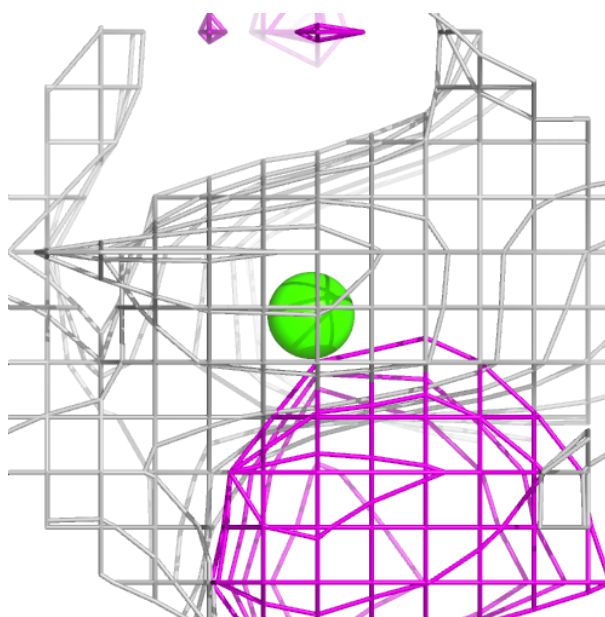
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	1501	1/1	0.86	0.20	111,111,111,111	0
2	CA	A	1502	1/1	0.86	0.33	122,122,122,122	0
2	CA	B	1501	1/1	0.90	0.22	135,135,135,135	0
2	CA	B	1502	1/1	0.94	0.12	133,133,133,133	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.

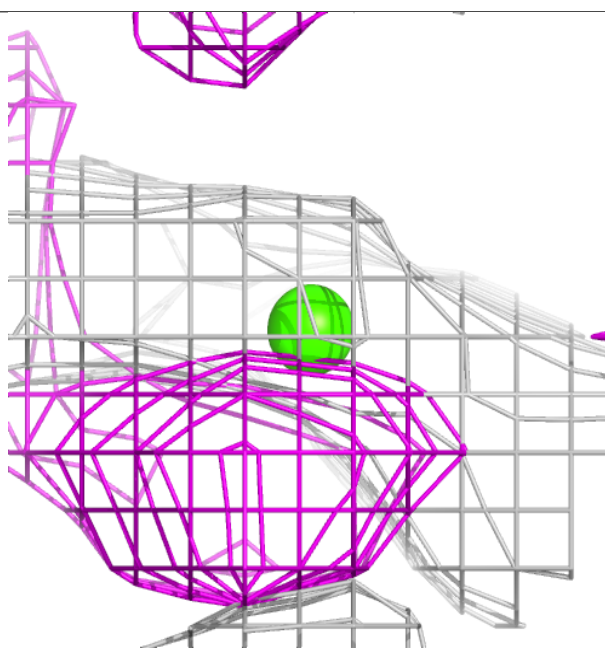
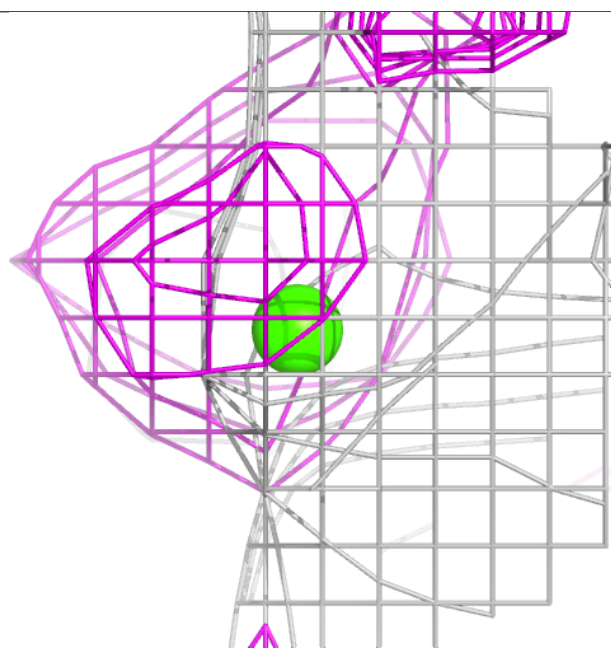
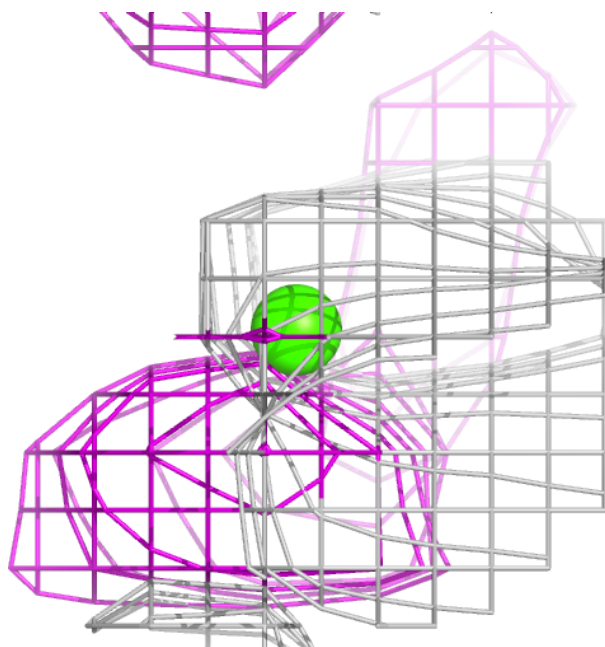
Electron density around CA A 1501:

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



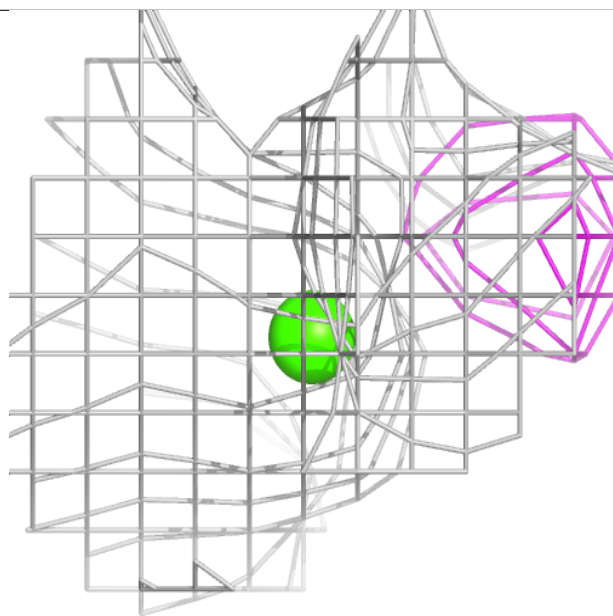
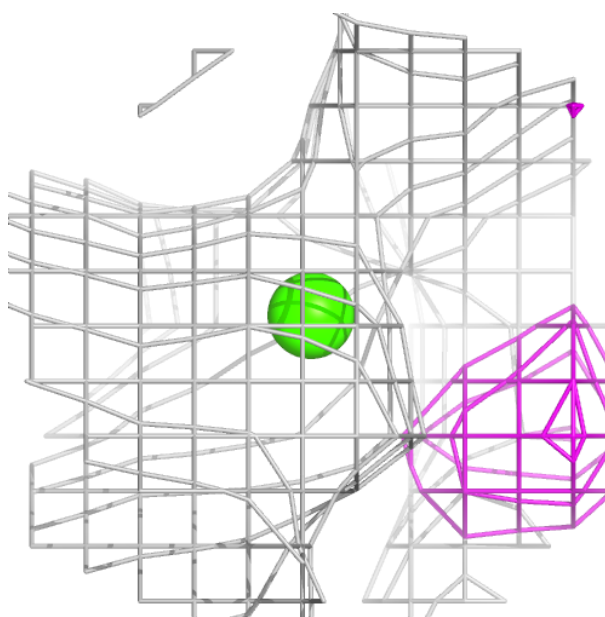
Electron density around CA A 1502:

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



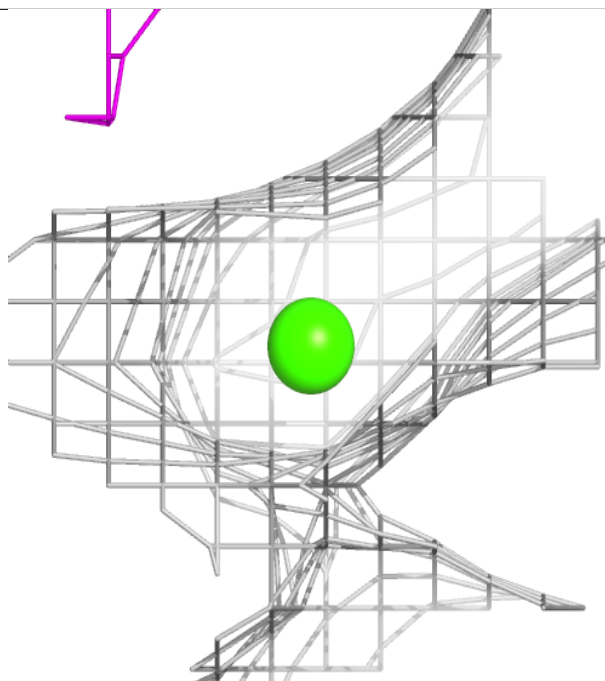
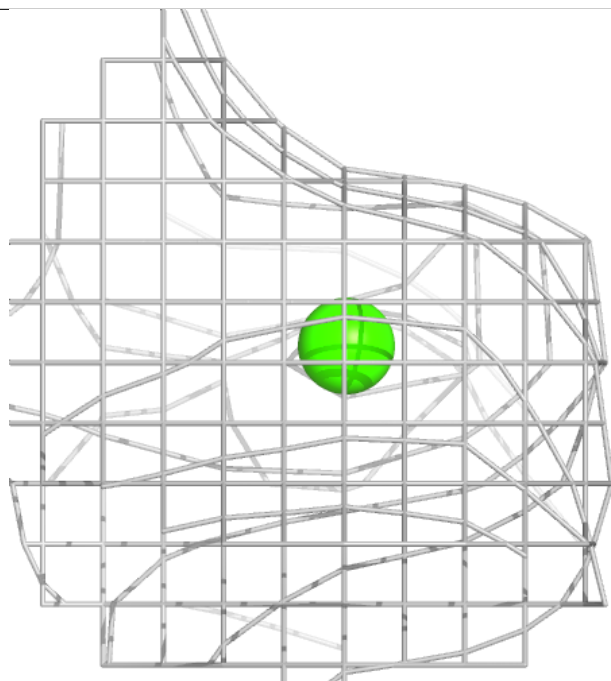
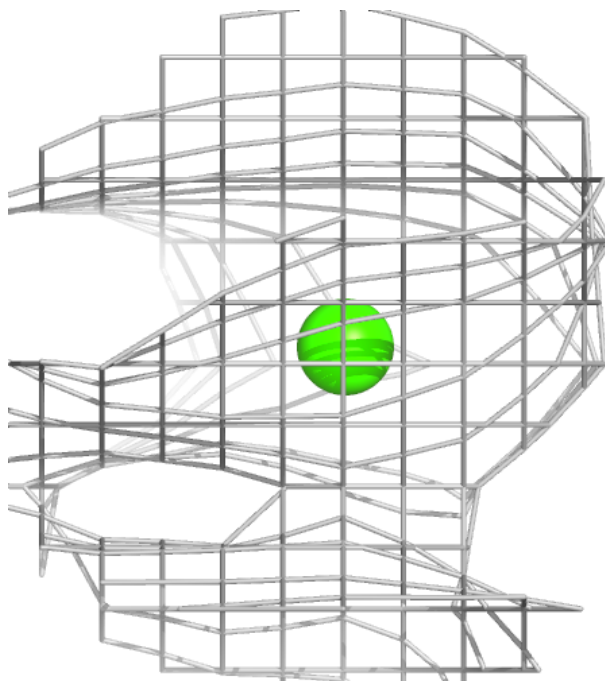
Electron density around CA B 1501:

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



Electron density around CA B 1502:

$2mF_o - DF_c$ (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.