



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2026 – 03:05 pm BST

PDB ID : 9RTS / pdb_00009rts
Title : Crystal structure of BRAF:MEK1(pS222) complex with asymmetric dimer interface bound to ADP
Authors : Kondo, Y.; Notbohm, J.; Camacho, I.N.; Nagy-Davidescu, G.; Mason, T.; Muhle, J.; Standfuss, J.; Perica, T.
Deposited on : 2025-07-03
Resolution : 2.30 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
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

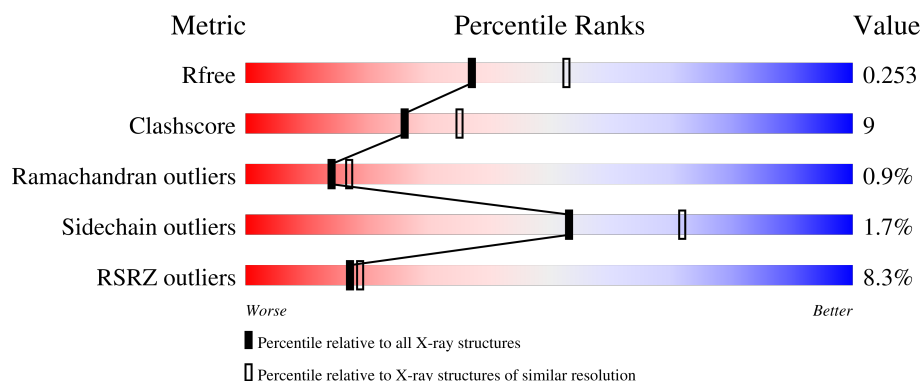
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	332	
1	D	332	
2	B	282	
2	C	282	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9218 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 Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	3	0
			2267	1451	381	417	1	17			
1	D	286	Total	C	N	O	P	S	0	0	0
			2243	1435	377	413	1	17			

- Molecule 2 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	273	Total	C	N	O	S	0	5	0
			2211	1401	391	406	13			
2	B	277	Total	C	N	O	S	0	1	0
			2231	1413	398	407	13			

There are 36 discrepancies between the modelled and reference sequences:

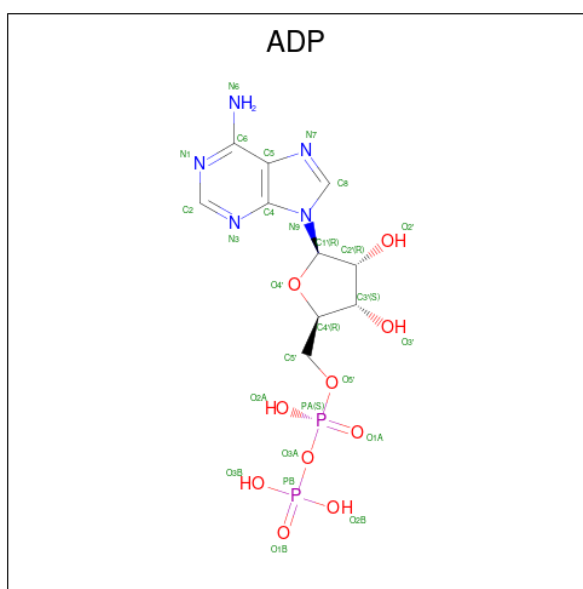
Chain	Residue	Modelled	Actual	Comment	Reference
C	442	SER	-	expression tag	UNP P15056
C	443	ASN	-	expression tag	UNP P15056
C	444	ALA	-	expression tag	UNP P15056
C	543	ALA	ILE	engineered mutation	UNP P15056
C	544	SER	ILE	engineered mutation	UNP P15056
C	551	LYS	ILE	engineered mutation	UNP P15056
C	562	ARG	GLN	engineered mutation	UNP P15056
C	588	ASN	LEU	engineered mutation	UNP P15056
C	600	GLU	VAL	conflict	UNP P15056
C	630	SER	LYS	engineered mutation	UNP P15056
C	688	ARG	ALA	engineered mutation	UNP P15056
C	706	SER	LEU	engineered mutation	UNP P15056
C	709	ARG	GLN	conflict	UNP P15056
C	713	GLU	SER	engineered mutation	UNP P15056
C	716	GLU	LEU	engineered mutation	UNP P15056
C	720	GLU	SER	engineered mutation	UNP P15056

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	722	SER	-	expression tag	UNP P15056
C	723	GLY	-	expression tag	UNP P15056
B	442	SER	-	expression tag	UNP P15056
B	443	ASN	-	expression tag	UNP P15056
B	444	ALA	-	expression tag	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	SER	ILE	engineered mutation	UNP P15056
B	551	LYS	ILE	engineered mutation	UNP P15056
B	562	ARG	GLN	engineered mutation	UNP P15056
B	588	ASN	LEU	engineered mutation	UNP P15056
B	600	GLU	VAL	conflict	UNP P15056
B	630	SER	LYS	engineered mutation	UNP P15056
B	688	ARG	ALA	engineered mutation	UNP P15056
B	706	SER	LEU	engineered mutation	UNP P15056
B	709	ARG	GLN	conflict	UNP P15056
B	713	GLU	SER	engineered mutation	UNP P15056
B	716	GLU	LEU	engineered mutation	UNP P15056
B	720	GLU	SER	engineered mutation	UNP P15056
B	722	SER	-	expression tag	UNP P15056
B	723	GLY	-	expression tag	UNP P15056

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

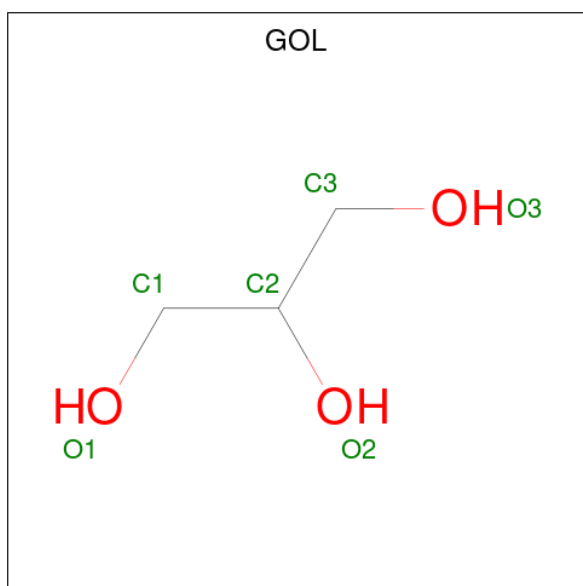
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Na 1	0	0

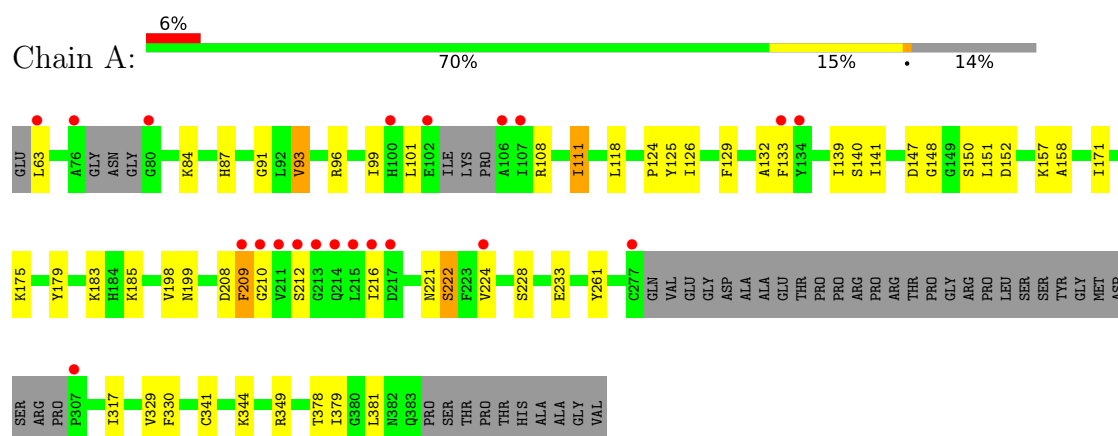
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	57	Total 57	O 57	0	0
7	C	42	Total 42	O 42	0	0
7	B	38	Total 38	O 38	0	0
7	D	6	Total 6	O 6	0	0

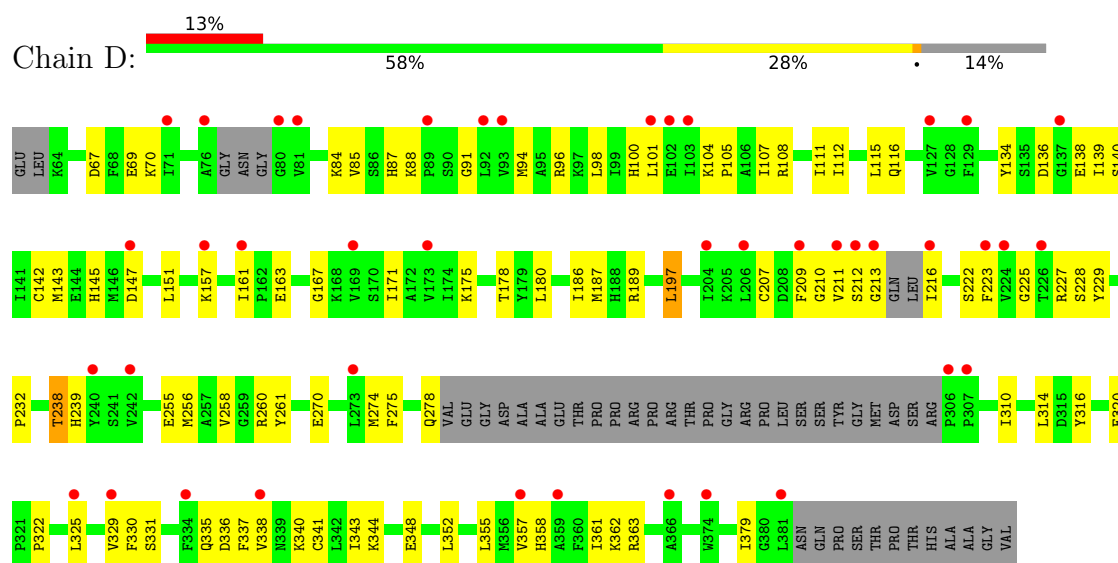
3 Residue-property plots [i](#)

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.

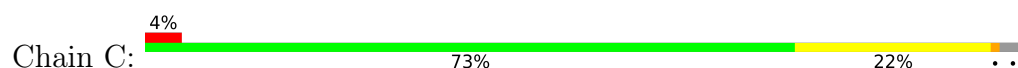
- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

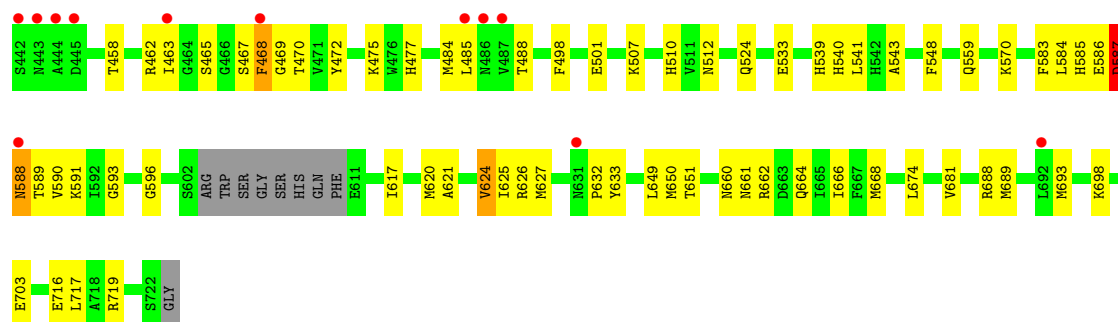


- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

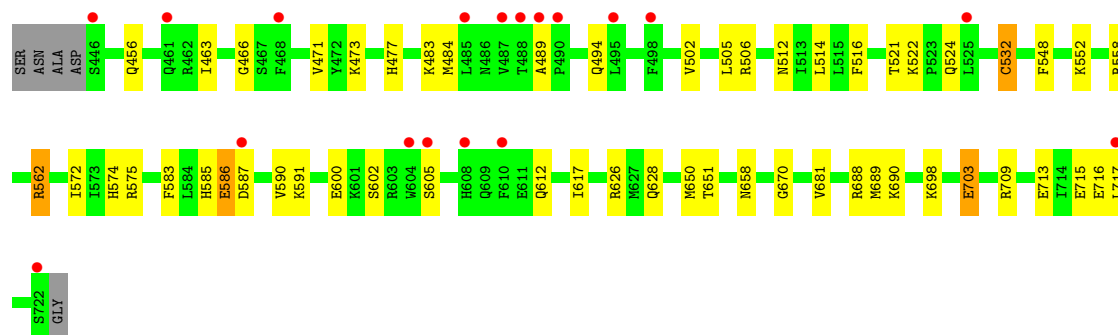
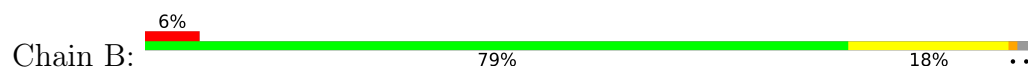


- Molecule 2: Serine/threonine-protein kinase B-raf





• Molecule 2: Serine/threonine-protein kinase B-raf



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.03Å 68.15Å 291.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 2.30 49.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	78.8 (49.75-2.30) 78.8 (49.75-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.211 , 0.253 0.211 , 0.253	Depositor DCC
R_{free} test set	1997 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9218	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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, SEP, NA, GOL, ADP

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	0.18	0/2310	0.38	0/3107
1	D	0.15	0/2278	0.34	0/3066
2	B	0.18	0/2283	0.38	0/3076
2	C	0.18	0/2271	0.41	2/3058 (0.1%)
All	All	0.17	0/9142	0.38	2/12307 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	587	ASP	CA-C-N	5.17	131.42	121.54
2	C	587	ASP	C-N-CA	5.17	131.42	121.54

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	2267	0	2289	35	0
1	D	2243	0	2263	60	1
2	B	2231	0	2235	35	0
2	C	2211	0	2228	48	1
3	A	27	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	6	0	8	0	0
6	B	1	0	0	0	0
7	A	57	0	0	2	0
7	B	38	0	0	1	0
7	C	42	0	0	2	0
7	D	6	0	0	0	0
All	All	9218	0	9071	170	1

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 (170) 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)
2:B:489:ALA:O	2:B:494:GLN:NE2	2.09	0.86
1:A:150:SER:OG	1:A:152:ASP:OD1	2.07	0.72
2:B:602:SER:H	2:B:605:SER:HB3	1.53	0.71
2:C:661[B]:ASN:ND2	7:C:1002:HOH:O	2.24	0.70
1:A:148:GLY:HA3	1:A:198:VAL:HG23	1.75	0.68
2:C:465:SER:HB2	1:D:136:ASP:HB3	1.76	0.67
2:C:541:LEU:HD11	2:C:649:LEU:HD23	1.78	0.65
1:D:161:ILE:HD12	1:D:256:MET:HE2	1.78	0.65
1:D:270:GLU:HG2	1:D:274:MET:HE2	1.79	0.65
1:D:145:HIS:NE2	1:D:147:ASP:OD1	2.29	0.64
2:C:512:ASN:HD21	2:C:559:GLN:HE21	1.46	0.64
2:C:681:VAL:HG11	2:C:693:MET:HE1	1.79	0.64
2:C:617:ILE:HA	2:C:620:MET:HE2	1.78	0.63
1:D:260:ARG:NH1	1:D:270:GLU:OE1	2.31	0.63
1:A:129[B]:PHE:HZ	1:A:132:ALA:HB2	1.63	0.63
2:C:540:HIS:HB3	2:C:548:PHE:HE2	1.65	0.61
1:D:101:LEU:HD12	1:D:139:ILE:HG13	1.82	0.61
1:A:157:LYS:HD2	1:A:379:ILE:HD12	1.84	0.60
1:A:233:GLU:OE2	1:A:349:ARG:NH2	2.35	0.59
1:D:232:PRO:HG3	1:D:344:LYS:HD2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:ARG:HH22	2:B:716:GLU:HG2	1.67	0.59
2:B:471:VAL:HG22	2:B:483:LYS:HG2	1.84	0.59
2:C:620:MET:HE3	2:C:625:ILE:HG12	1.84	0.59
1:D:108:ARG:HD2	1:D:134:TYR:CE2	2.38	0.59
2:C:462:ARG:NH2	2:C:469:GLY:O	2.35	0.58
2:B:650:MET:HE3	2:B:689:MET:HG2	1.84	0.58
2:B:626:ARG:HB3	2:B:628:GLN:HG3	1.85	0.57
1:A:129[B]:PHE:HE1	1:A:141:ILE:HG23	1.68	0.57
2:B:698:LYS:HD3	2:B:703:GLU:HB3	1.87	0.57
1:D:325:LEU:HG	1:D:338:VAL:HG21	1.87	0.57
2:C:650:MET:HE3	2:C:689:MET:HG2	1.86	0.57
1:A:84:LYS:HE3	1:A:93:VAL:HG21	1.87	0.56
2:C:698:LYS:HD3	2:C:703:GLU:HB3	1.87	0.56
1:D:187:MET:HE2	1:D:189:ARG:HG2	1.86	0.56
1:A:101:LEU:HD11	1:A:139:ILE:HD11	1.86	0.56
1:A:212:SER:OG	7:A:1001:HOH:O	2.18	0.56
2:C:688:ARG:HD3	2:C:717:LEU:HD13	1.88	0.55
2:B:521:THR:HG23	2:B:522:LYS:HG3	1.88	0.55
1:A:87:HIS:O	1:A:91:GLY:N	2.40	0.55
1:D:336:ASP:OD2	1:D:358:HIS:NE2	2.34	0.54
1:D:212:SER:HA	1:D:216:ILE:HG12	1.89	0.54
2:C:661[B]:ASN:HB2	2:C:664:GLN:HB3	1.90	0.54
2:C:586:GLU:C	2:C:588:ASN:H	2.17	0.53
1:D:151:LEU:HD13	1:D:256:MET:HE1	1.89	0.53
2:B:463:ILE:HD11	2:B:473:LYS:HB2	1.88	0.53
2:B:651:THR:HG22	2:B:681:VAL:HA	1.90	0.53
1:D:171:ILE:HG22	1:D:175:LYS:HE2	1.91	0.53
2:C:507:LYS:O	2:C:570:LYS:NZ	2.31	0.53
2:C:468:PHE:CG	1:D:100:HIS:HB2	2.44	0.53
2:B:514:LEU:HD11	2:B:583:PHE:HE2	1.74	0.53
1:D:238:THR:HG22	1:D:239:HIS:H	1.73	0.53
2:B:484:MET:HE1	2:B:524:GLN:HB3	1.91	0.53
1:A:96:ARG:HE	1:A:140:SER:HB2	1.74	0.52
1:D:105:PRO:HA	1:D:108:ARG:NE	2.24	0.52
1:A:129[B]:PHE:CE1	1:A:141:ILE:HG23	2.45	0.52
1:D:105:PRO:HA	1:D:108:ARG:HE	1.74	0.52
2:C:661[A]:ASN:HB3	2:C:664:GLN:HB3	1.92	0.52
1:D:151:LEU:HB3	1:D:256:MET:HE1	1.92	0.52
2:C:533:GLU:H	2:C:585:HIS:CE1	2.28	0.51
1:D:96:ARG:NH2	1:D:140:SER:OG	2.41	0.51
2:C:617:ILE:HD13	2:C:662:ARG:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLY:O	1:D:171:ILE:HG12	2.10	0.51
2:C:626:ARG:NH1	7:C:1007:HOH:O	2.43	0.51
2:B:585:HIS:C	2:B:587:ASP:H	2.19	0.51
1:A:158:ALA:HB2	1:A:378:THR:HG21	1.93	0.50
2:C:510:HIS:CD2	2:B:456:GLN:HE22	2.29	0.50
2:C:651:THR:HG22	2:C:681:VAL:HA	1.92	0.50
2:C:484:MET:SD	2:C:524:GLN:NE2	2.83	0.50
1:D:322:PRO:HG3	1:D:344:LYS:HG2	1.93	0.50
1:D:163:GLU:OE2	1:D:331:SER:OG	2.22	0.50
2:C:477:HIS:CE1	2:B:591:LYS:HE3	2.46	0.50
1:D:98:LEU:HD12	1:D:138:GLU:HB3	1.94	0.50
2:C:591:LYS:HE3	2:B:477:HIS:CE1	2.47	0.49
2:B:489:ALA:C	2:B:494:GLN:HE22	2.14	0.49
1:D:94:MET:HE1	1:D:142:CYS:HB3	1.93	0.49
2:B:574:HIS:O	2:B:575:ARG:HB2	2.13	0.49
2:C:468:PHE:CD2	1:D:100:HIS:HB2	2.46	0.49
2:C:624:VAL:HA	2:C:632:PRO:HB2	1.95	0.49
1:A:224:VAL:HG22	2:B:617:ILE:HD11	1.95	0.49
1:D:343:ILE:HG21	1:D:348:GLU:HB2	1.95	0.49
1:A:329:VAL:HG23	1:A:330:PHE:CD2	2.48	0.48
2:C:462:ARG:HH12	2:C:465:SER:C	2.21	0.48
1:D:143:MET:HE2	3:D:901:ADP:HN61	1.77	0.48
2:C:485:LEU:HD12	2:C:498:PHE:HB2	1.95	0.48
1:D:329:VAL:HG23	1:D:330:PHE:CD2	2.49	0.48
1:A:126:ILE:HG23	1:A:209:PHE:CZ	2.49	0.48
2:B:548:PHE:CD1	2:B:552:LYS:HD3	2.49	0.48
1:A:63:LEU:HD22	1:A:133:PHE:HB2	1.96	0.48
1:D:180:LEU:HD22	1:D:186:ILE:HD11	1.96	0.48
1:D:357:VAL:HA	1:D:362:LYS:HE3	1.95	0.47
1:D:70:LYS:HA	1:D:85:VAL:HG12	1.96	0.47
1:D:209:PHE:O	1:D:211:VAL:N	2.38	0.47
1:D:337:PHE:CE1	1:D:355:LEU:HD22	2.50	0.47
1:D:316:TYR:CD2	1:D:320:GLU:HG3	2.50	0.47
1:D:171:ILE:HD13	1:D:361:ILE:HD12	1.97	0.47
1:A:99:ILE:HB	1:A:139:ILE:HB	1.97	0.47
1:D:104:LYS:HD3	1:D:107:ILE:HD13	1.95	0.46
1:A:228:SER:O	1:A:261:TYR:OH	2.23	0.46
1:D:278:GLN:HG3	1:D:329:VAL:HG13	1.97	0.46
2:B:552:LYS:NZ	2:B:587:ASP:O	2.26	0.46
2:B:505:LEU:HB3	2:B:516:PHE:CG	2.50	0.46
1:D:209:PHE:C	1:D:211:VAL:H	2.22	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASP:OD1	7:A:1001:HOH:O	2.20	0.45
2:B:585:HIS:O	2:B:587:ASP:N	2.50	0.45
1:A:147:ASP:HB3	1:A:381:LEU:HD13	1.98	0.45
1:A:341:CYS:O	1:A:349:ARG:HD2	2.17	0.45
2:C:559:GLN:NE2	2:C:590:VAL:H	2.14	0.45
2:B:514:LEU:HD11	2:B:583:PHE:CE2	2.52	0.45
1:A:171:ILE:HG22	1:A:175:LYS:HE2	1.99	0.45
1:A:221:ASN:OD1	1:A:222:SEP:N	2.50	0.45
2:B:572:ILE:HG12	2:B:600:GLU:HG2	1.99	0.44
2:C:716:GLU:O	2:C:719:ARG:HG2	2.18	0.44
2:B:658:ASN:HB2	7:B:1015:HOH:O	2.16	0.44
1:D:336:ASP:OD1	1:D:340:LYS:NZ	2.49	0.44
1:A:108:ARG:O	1:A:111:ILE:HG13	2.18	0.44
2:C:458:THR:OG1	2:C:475:LYS:HB2	2.17	0.44
2:B:585:HIS:C	2:B:587:ASP:N	2.74	0.44
1:D:363:ARG:NH1	1:D:363:ARG:HB2	2.33	0.44
2:C:539:HIS:HA	2:C:543:ALA:HB3	2.00	0.44
1:A:126:ILE:HG23	1:A:209:PHE:HZ	1.82	0.43
2:C:585:HIS:O	2:C:588:ASN:N	2.51	0.43
1:D:258:VAL:HG13	1:D:275:PHE:HZ	1.83	0.43
2:C:470:THR:HB	2:C:484:MET:O	2.18	0.43
2:C:583[B]:PHE:HE2	2:C:593:GLY:HA3	1.83	0.43
2:B:688:ARG:NH1	2:B:713:GLU:OE1	2.51	0.43
1:D:104:LYS:O	1:D:108:ARG:HG3	2.19	0.43
1:D:227:ARG:NH1	1:D:255:GLU:OE2	2.51	0.43
2:C:627:MET:HE1	2:C:633:TYR:CE2	2.53	0.43
1:D:112:ILE:O	1:D:116:GLN:HG2	2.19	0.43
2:B:626:ARG:NH1	2:B:670:GLY:O	2.45	0.43
1:D:310:ILE:O	1:D:314:LEU:HG	2.18	0.43
1:A:96:ARG:HH21	1:A:140:SER:HB3	1.84	0.42
2:C:462:ARG:HD2	2:C:472:TYR:CZ	2.54	0.42
1:A:133:PHE:HB3	1:A:140:SER:OG	2.19	0.42
1:D:151:LEU:HD23	1:D:151:LEU:HA	1.84	0.42
1:D:325:LEU:HD12	1:D:335:GLN:HA	2.00	0.42
2:C:540:HIS:ND1	2:C:584:LEU:HD12	2.35	0.42
2:C:587:ASP:C	2:C:589:THR:H	2.27	0.42
1:D:178:THR:HG22	1:D:352:LEU:HD13	2.02	0.42
2:C:660:ASN:HB2	1:D:213:GLY:C	2.45	0.42
1:D:157:LYS:HD2	1:D:379:ILE:CD1	2.50	0.42
1:D:197:LEU:HD21	1:D:207:CYS:SG	2.60	0.42
2:C:540:HIS:HB3	2:C:548:PHE:CE2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:HIS:O	1:D:91:GLY:N	2.53	0.42
2:B:512:ASN:OD1	2:B:562:ARG:NH1	2.53	0.42
2:B:558:ARG:HD2	2:B:715:GLU:HG2	2.02	0.42
1:D:84:LYS:HD2	1:D:145:HIS:CE1	2.54	0.42
2:C:625:ILE:HG23	2:C:666:ILE:HG23	2.02	0.41
2:B:681:VAL:HG21	2:B:690:LYS:HD2	2.02	0.41
1:D:151:LEU:HB3	1:D:256:MET:CE	2.50	0.41
1:A:124:PRO:HG2	1:A:125:TYR:CE2	2.55	0.41
1:D:108:ARG:O	1:D:112:ILE:HG12	2.20	0.41
1:A:179:TYR:CE1	1:A:183:LYS:HG3	2.56	0.41
1:A:317:ILE:O	1:A:344:LYS:HE2	2.20	0.41
1:D:111:ILE:O	1:D:115:LEU:HG	2.20	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.84	0.41
2:C:621:ALA:HB3	2:C:624:VAL:HG13	2.03	0.41
2:B:532:CYS:SG	2:B:585:HIS:HB2	2.61	0.41
2:B:502:VAL:O	2:B:506:ARG:HG3	2.21	0.41
1:A:101:LEU:HD21	1:A:216:ILE:HG22	2.03	0.41
2:C:501:GLU:HB2	2:C:596:GLY:HA2	2.03	0.41
1:A:148:GLY:H	1:A:199:ASN:HA	1.87	0.40
2:C:512:ASN:ND2	2:C:559:GLN:HE21	2.13	0.40
1:D:228:SER:O	1:D:261:TYR:OH	2.30	0.40
1:D:69:GLU:HB2	1:D:88:LYS:HE3	2.04	0.40
1:D:229:TYR:OH	1:D:255:GLU:OE1	2.27	0.40
2:C:668:MET:HE3	2:C:674:LEU:HD22	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:588:ASN:ND2	1:D:67:ASP:OD1[3_445]	2.16	0.04

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	280/332 (84%)	274 (98%)	5 (2%)	1 (0%)	30	38
1	D	277/332 (83%)	268 (97%)	7 (2%)	2 (1%)	18	23
2	B	276/282 (98%)	266 (96%)	8 (3%)	2 (1%)	18	23
2	C	274/282 (97%)	260 (95%)	9 (3%)	5 (2%)	6	6
All	All	1107/1228 (90%)	1068 (96%)	29 (3%)	10 (1%)	14	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	225	GLY
1	A	210	GLY
2	C	587	ASP
1	D	210	GLY
2	C	468	PHE
2	C	488	THR
2	B	586	GLU
2	C	467	SER
2	C	588	ASN
2	B	466	GLY

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	251/284 (88%)	247 (98%)	4 (2%)	55	73
1	D	248/284 (87%)	244 (98%)	4 (2%)	55	73
2	B	245/247 (99%)	238 (97%)	7 (3%)	37	55
2	C	245/247 (99%)	243 (99%)	2 (1%)	73	86
All	All	989/1062 (93%)	972 (98%)	17 (2%)	53	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	A	111	ILE
1	A	118	LEU
1	A	209	PHE
2	C	463	ILE
2	C	624	VAL
2	B	532	CYS
2	B	562	ARG
2	B	586	GLU
2	B	590	VAL
2	B	612	GLN
2	B	703	GLU
2	B	717	LEU
1	D	197	LEU
1	D	223	PHE
1	D	238	THR
1	D	341	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	145	HIS
1	A	184	HIS
2	C	496	GLN
2	C	559	GLN
2	C	585	HIS
2	B	493	GLN
2	B	496	GLN
2	B	653	GLN
1	D	87	HIS
1	D	100	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	SEP	A	222	1	8,9,10	1.60	1 (12%)	8,12,14	1.46	2 (25%)
1	SEP	D	222	1	8,9,10	1.59	1 (12%)	8,12,14	1.54	2 (25%)

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
1	SEP	A	222	1	-	0/5/8/10	-
1	SEP	D	222	1	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	SEP	P-O1P	3.50	1.61	1.50
1	D	222	SEP	P-O1P	3.46	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	222	SEP	P-OG-CB	-3.02	109.97	118.30
1	A	222	SEP	P-OG-CB	-2.84	110.47	118.30
1	D	222	SEP	OG-CB-CA	2.73	110.80	108.14
1	A	222	SEP	OG-CB-CA	2.45	110.53	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	222	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	222	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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$
5	GOL	A	904	-	5,5,5	0.96	0	5,5,5	0.97	0
3	ADP	A	901	4	27,29,29	1.36	4 (14%)	42,45,45	1.93	10 (23%)
3	ADP	B	901	4	27,29,29	1.35	4 (14%)	42,45,45	1.96	12 (28%)
3	ADP	C	901	4	27,29,29	1.35	4 (14%)	42,45,45	1.94	12 (28%)
3	ADP	D	901	4	27,29,29	1.37	4 (14%)	42,45,45	1.92	10 (23%)

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
5	GOL	A	904	-	-	2/4/4/4	-
3	ADP	A	901	4	-	3/16/32/32	0/3/3/3
3	ADP	B	901	4	-	2/16/32/32	0/3/3/3
3	ADP	C	901	4	-	2/16/32/32	0/3/3/3
3	ADP	D	901	4	-	4/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	ADP	C5-C4	4.66	1.47	1.39
3	C	901	ADP	C5-C4	4.51	1.47	1.39
3	A	901	ADP	C5-C4	4.49	1.47	1.39
3	B	901	ADP	C5-C4	4.49	1.47	1.39
3	A	901	ADP	C5-C6	2.76	1.48	1.41
3	D	901	ADP	C5-C6	2.70	1.48	1.41
3	C	901	ADP	C5-C6	2.68	1.48	1.41
3	B	901	ADP	C5-C6	2.66	1.48	1.41
3	A	901	ADP	C8-N7	2.54	1.36	1.31
3	C	901	ADP	C8-N7	2.52	1.36	1.31
3	B	901	ADP	C8-N7	2.43	1.36	1.31
3	D	901	ADP	C8-N7	2.36	1.36	1.31
3	A	901	ADP	C5-N7	-2.20	1.34	1.39
3	D	901	ADP	C5-N7	-2.15	1.35	1.39
3	B	901	ADP	C5-N7	-2.07	1.35	1.39
3	C	901	ADP	C5-N7	-2.06	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ADP	C5-C4-N3	-6.40	118.40	126.75
3	D	901	ADP	C5-C4-N3	-6.22	118.64	126.75
3	C	901	ADP	C5-C4-N3	-6.14	118.74	126.75
3	B	901	ADP	C5-C4-N3	-5.99	118.93	126.75
3	D	901	ADP	N3-C4-N9	4.92	135.19	127.08
3	A	901	ADP	N3-C4-N9	4.81	135.01	127.08
3	B	901	ADP	N3-C4-N9	4.71	134.84	127.08
3	C	901	ADP	N3-C4-N9	4.68	134.80	127.08
3	A	901	ADP	C2-N3-C4	3.91	120.99	111.75
3	B	901	ADP	C2-N3-C4	3.85	120.84	111.75
3	D	901	ADP	C2-N3-C4	3.82	120.78	111.75
3	C	901	ADP	C2-N3-C4	3.82	120.76	111.75
3	A	901	ADP	C4-C5-N7	-3.53	106.32	110.62
3	C	901	ADP	C4-C5-N7	-3.32	106.58	110.62
3	B	901	ADP	N3-C2-N1	-3.27	123.49	128.60
3	B	901	ADP	C4-C5-N7	-3.25	106.66	110.62
3	D	901	ADP	C4-C5-N7	-3.14	106.79	110.62
3	D	901	ADP	N3-C2-N1	-3.08	123.78	128.60
3	C	901	ADP	N3-C2-N1	-3.00	123.91	128.60
3	A	901	ADP	C5-N7-C8	2.99	107.75	103.51
3	A	901	ADP	N3-C2-N1	-2.96	123.97	128.60
3	D	901	ADP	PA-O3A-PB	-2.86	123.01	132.83
3	B	901	ADP	C5-N7-C8	2.81	107.51	103.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	ADP	C4-N9-C8	2.73	108.69	105.73
3	C	901	ADP	C5-N7-C8	2.71	107.36	103.51
3	B	901	ADP	C2'-C1'-N9	-2.66	106.57	113.30
3	C	901	ADP	C2'-C1'-N9	-2.64	106.62	113.30
3	A	901	ADP	C3'-C2'-C1'	2.63	106.43	101.43
3	D	901	ADP	C5-N7-C8	2.63	107.25	103.51
3	B	901	ADP	C3'-C2'-C1'	2.60	106.37	101.43
3	C	901	ADP	C4-N9-C8	2.55	108.49	105.73
3	A	901	ADP	C4-N9-C8	2.51	108.45	105.73
3	D	901	ADP	C3'-C2'-C1'	2.45	106.09	101.43
3	D	901	ADP	C4-N9-C8	2.42	108.35	105.73
3	C	901	ADP	C3'-C2'-C1'	2.39	105.96	101.43
3	B	901	ADP	C6-C5-N7	2.31	136.33	132.02
3	B	901	ADP	PA-O3A-PB	-2.29	124.96	132.83
3	A	901	ADP	C6-C5-N7	2.26	136.24	132.02
3	C	901	ADP	C6-C5-N7	2.25	136.21	132.02
3	A	901	ADP	N9-C8-N7	-2.21	110.89	113.91
3	B	901	ADP	N9-C8-N7	-2.18	110.93	113.91
3	C	901	ADP	PA-O3A-PB	-2.07	125.71	132.83
3	C	901	ADP	N9-C8-N7	-2.05	111.11	113.91
3	D	901	ADP	C6-C5-N7	2.02	135.78	132.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

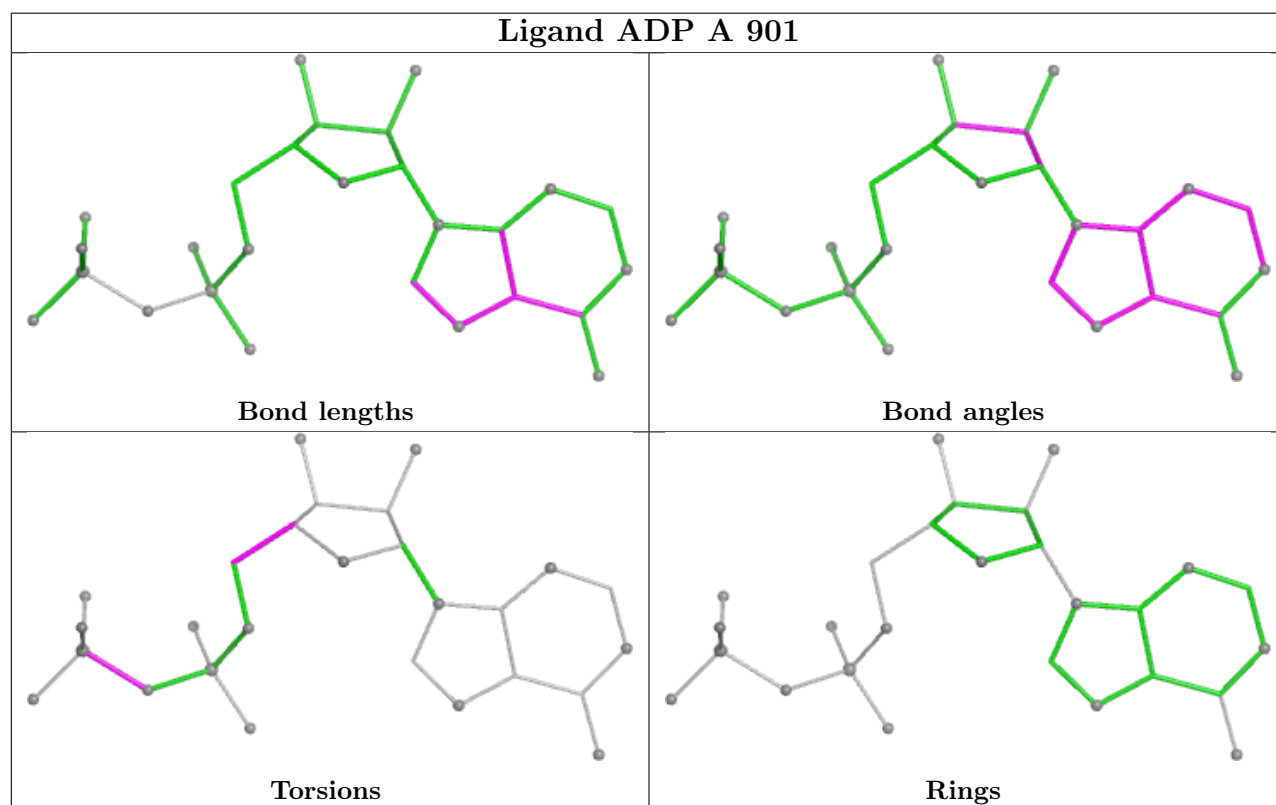
Mol	Chain	Res	Type	Atoms
3	A	901	ADP	PA-O3A-PB-O2B
3	D	901	ADP	C5'-O5'-PA-O1A
3	D	901	ADP	C5'-O5'-PA-O2A
3	D	901	ADP	C5'-O5'-PA-O3A
5	A	904	GOL	C1-C2-C3-O3
3	A	901	ADP	O4'-C4'-C5'-O5'
3	A	901	ADP	C3'-C4'-C5'-O5'
5	A	904	GOL	O2-C2-C3-O3
3	B	901	ADP	O4'-C4'-C5'-O5'
3	D	901	ADP	PB-O3A-PA-O2A
3	C	901	ADP	O4'-C4'-C5'-O5'
3	B	901	ADP	C3'-C4'-C5'-O5'
3	C	901	ADP	C3'-C4'-C5'-O5'

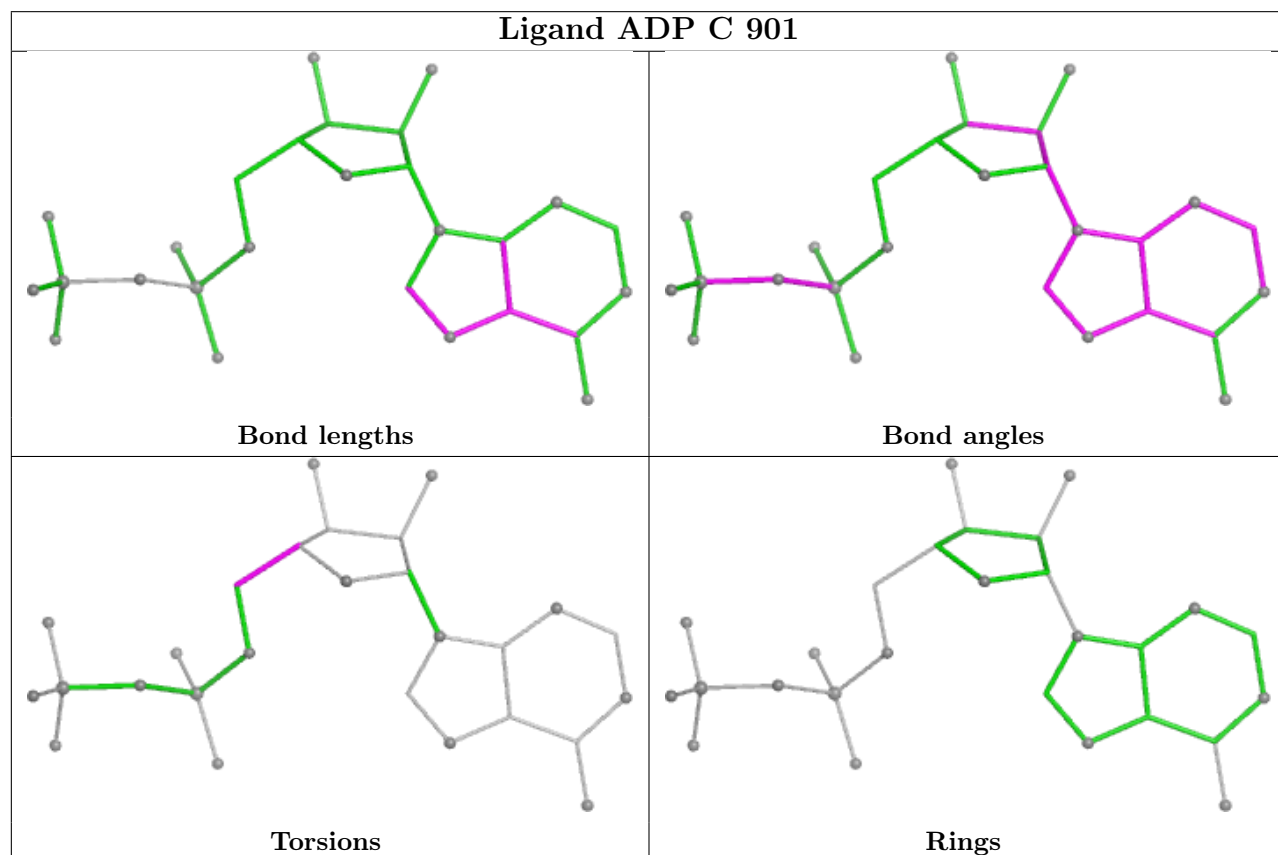
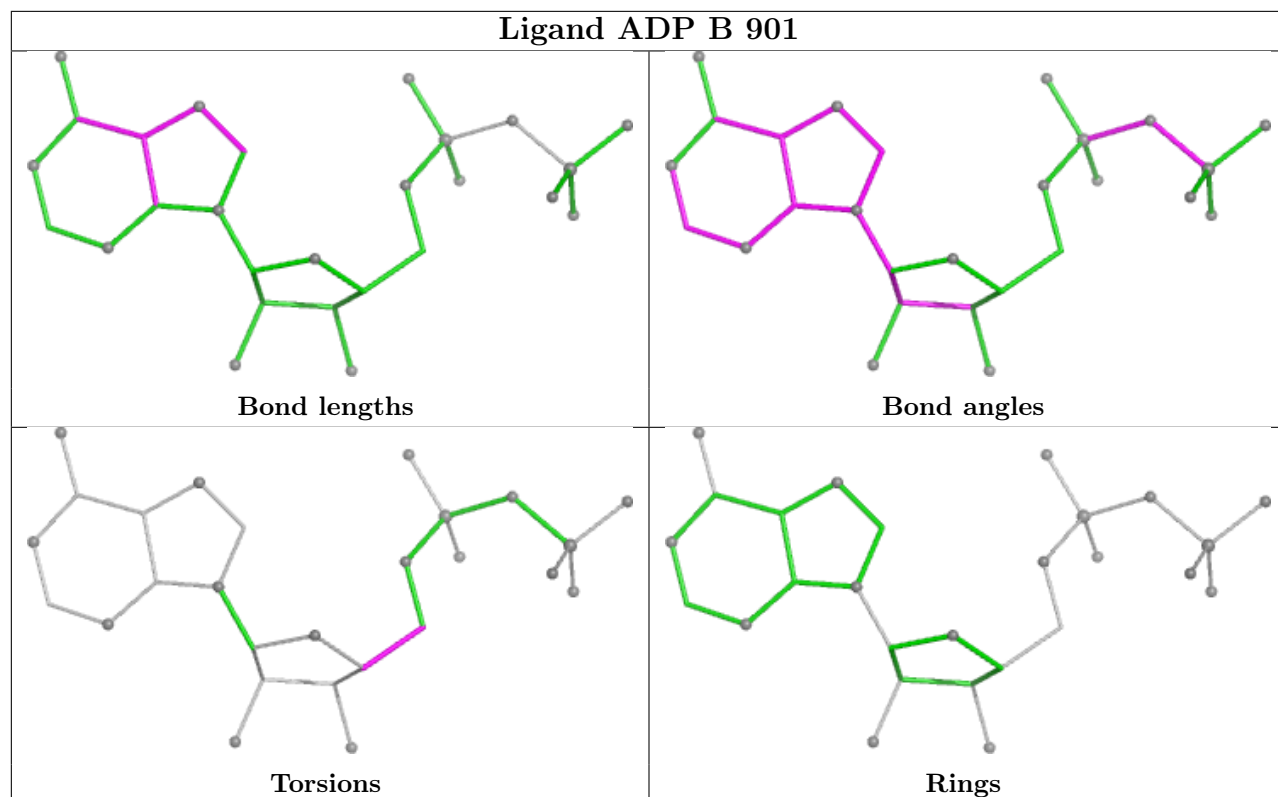
There are no ring outliers.

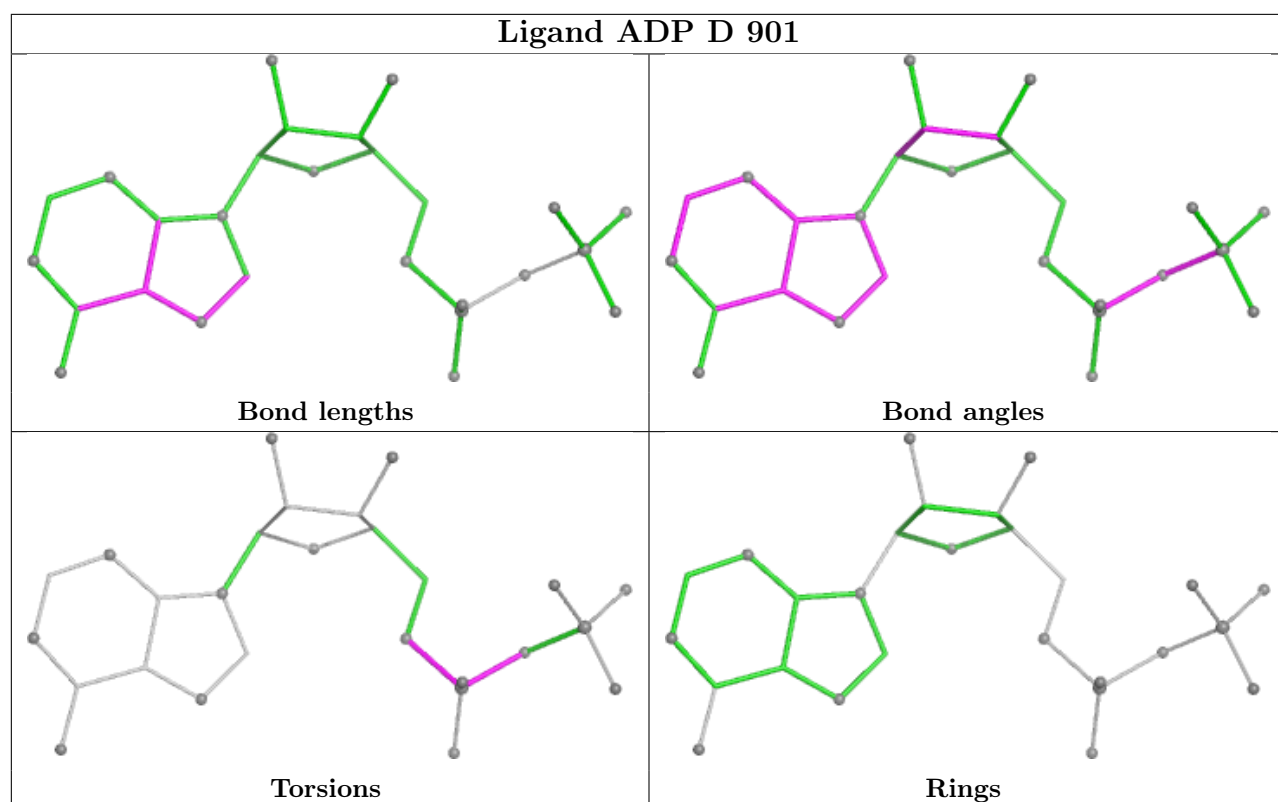
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	901	ADP	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	285/332 (85%)	0.36	21 (7%)	20 22	31, 63, 138, 192	3 (1%)
1	D	285/332 (85%)	1.01	42 (14%)	6 6	39, 119, 161, 184	0
2	B	277/282 (98%)	0.42	18 (6%)	25 27	34, 65, 127, 213	1 (0%)
2	C	273/282 (96%)	0.40	12 (4%)	39 41	27, 68, 131, 194	5 (1%)
All	All	1120/1228 (91%)	0.55	93 (8%)	17 19	27, 78, 150, 213	9 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	485	LEU	6.3
1	A	211	VAL	5.5
2	B	487	VAL	5.2
2	B	468	PHE	5.1
1	D	224	VAL	4.6
1	A	215	LEU	4.3
2	C	443	ASN	4.2
1	A	209	PHE	4.0
1	A	107	ILE	3.8
1	A	212	SER	3.7
1	D	329	VAL	3.7
2	B	525	LEU	3.6
1	D	80	GLY	3.6
2	C	445	ASP	3.6
1	A	213	GLY	3.5
1	A	210	GLY	3.4
1	A	134	TYR	3.4
2	C	486	ASN	3.4
1	D	381	LEU	3.3
1	D	223	PHE	3.3
1	D	242	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	224	VAL	3.2
2	B	608	HIS	3.2
1	D	211	VAL	3.1
1	A	307	PRO	3.1
1	D	92	LEU	3.1
1	D	127	VAL	3.0
1	D	76	ALA	3.0
1	D	93	VAL	3.0
1	A	106	ALA	2.9
2	B	461	GLN	2.9
2	B	604	TRP	2.9
1	A	76	ALA	2.9
1	D	213	GLY	2.9
1	D	334	PHE	2.9
1	D	216	ILE	2.9
1	D	161	ILE	2.9
2	C	444	ALA	2.8
1	A	216	ILE	2.8
1	D	273	LEU	2.8
1	D	374	TRP	2.8
1	D	169	VAL	2.8
1	D	103	ILE	2.8
1	D	357	VAL	2.7
2	B	495	LEU	2.6
2	C	631	ASN	2.6
2	B	498	PHE	2.6
1	D	359	ALA	2.6
1	D	129	PHE	2.6
1	D	325	LEU	2.6
1	D	306	PRO	2.6
2	C	442	SER	2.5
2	B	587	ASP	2.5
1	D	307	PRO	2.5
2	C	463	ILE	2.5
1	A	133	PHE	2.4
2	C	468	PHE	2.4
2	B	605	SER	2.4
1	D	71	ILE	2.4
1	D	173	VAL	2.4
1	A	80	GLY	2.4
1	D	157	LYS	2.4
1	D	209	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	240	TYR	2.3
1	D	338	VAL	2.3
2	C	487	VAL	2.3
2	B	717	LEU	2.3
2	B	610	PHE	2.3
1	D	101	LEU	2.3
1	A	100	HIS	2.3
2	B	485	LEU	2.3
1	A	217	ASP	2.3
2	B	488	THR	2.2
1	D	81	VAL	2.2
2	C	588	ASN	2.2
1	D	212	SER	2.2
2	B	446	SER	2.2
1	A	102	GLU	2.2
1	D	102	GLU	2.2
1	D	366	ALA	2.2
2	B	722	SER	2.2
1	A	277	CYS	2.1
1	D	204	ILE	2.1
1	A	214	GLN	2.1
1	D	89	PRO	2.1
2	B	490	PRO	2.1
1	D	137	GLY	2.1
1	D	206	LEU	2.1
2	C	692	LEU	2.0
1	D	226	THR	2.0
2	B	489	ALA	2.0
1	A	63	LEU	2.0
1	D	147	ASP	2.0

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

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
1	SEP	A	222	10/11	0.87	0.12	70,75,90,117	0
1	SEP	D	222	10/11	0.87	0.11	80,87,97,106	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

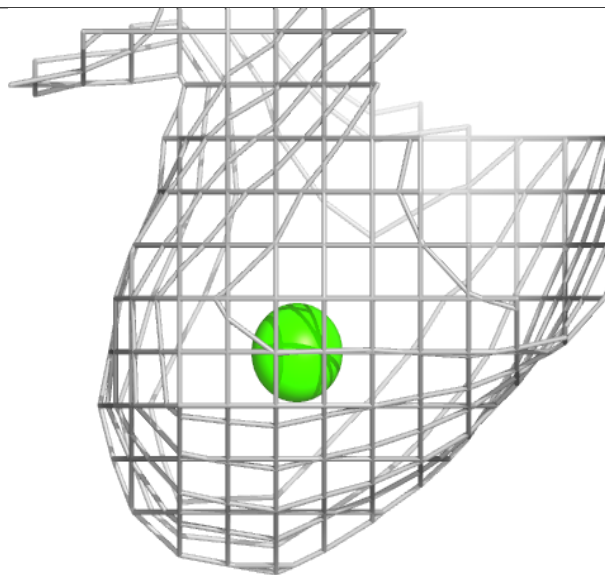
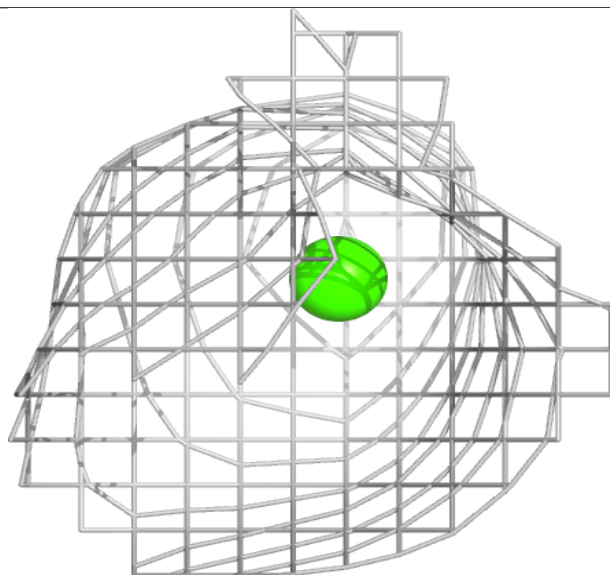
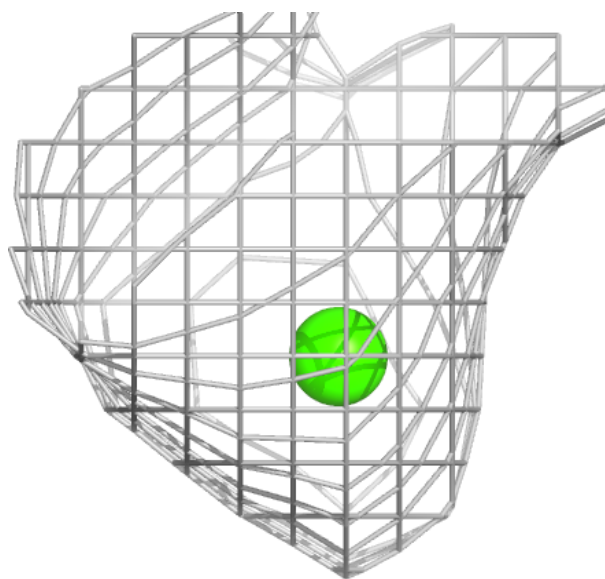
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	904	6/6	0.76	0.14	81,85,94,101	0
4	CA	D	903	1/1	0.83	0.11	117,117,117,117	0
6	NA	B	904	1/1	0.83	0.15	72,72,72,72	0
3	ADP	D	901	27/27	0.86	0.10	92,100,133,148	0
4	CA	B	902	1/1	0.93	0.05	76,76,76,76	0
3	ADP	B	901	27/27	0.94	0.08	45,62,73,97	0
3	ADP	A	901	27/27	0.94	0.08	44,64,80,85	0
3	ADP	C	901	27/27	0.94	0.08	54,67,78,94	0
4	CA	D	902	1/1	0.95	0.06	114,114,114,114	0
4	CA	A	902	1/1	0.95	0.10	78,78,78,78	0
4	CA	C	902	1/1	0.97	0.04	64,64,64,64	0
4	CA	A	903	1/1	0.98	0.04	76,76,76,76	0
4	CA	B	903	1/1	0.98	0.04	65,65,65,65	0
4	CA	C	903	1/1	0.99	0.03	63,63,63,63	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.

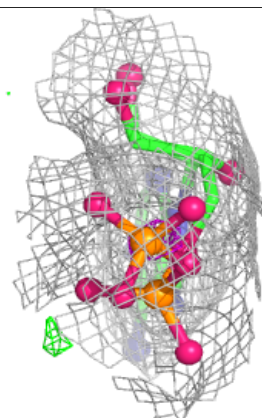
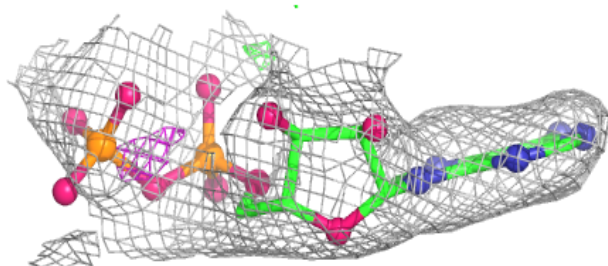
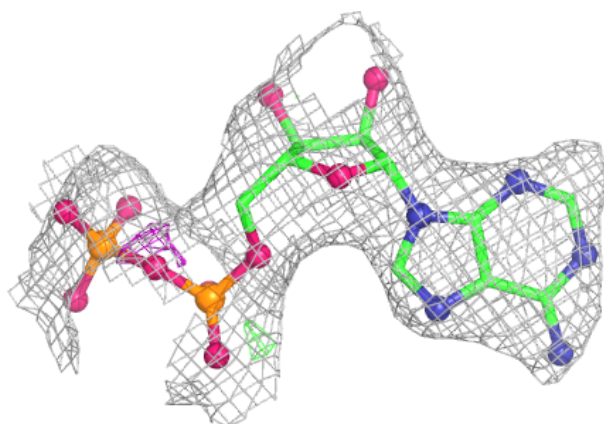
Electron density around CA D 903:

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



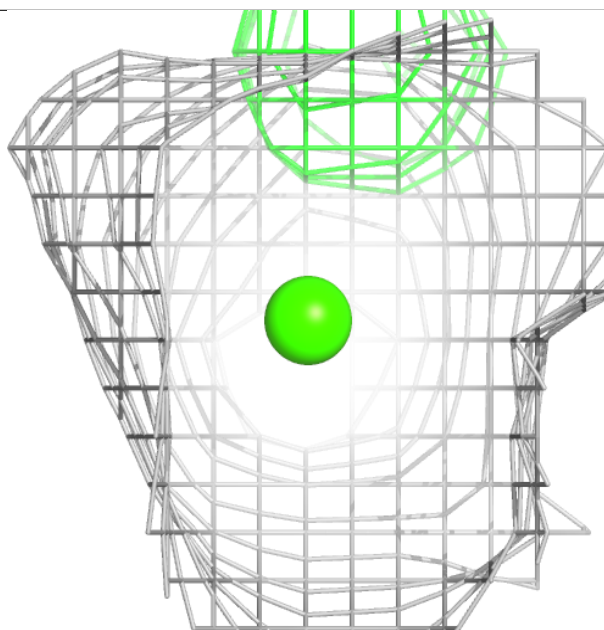
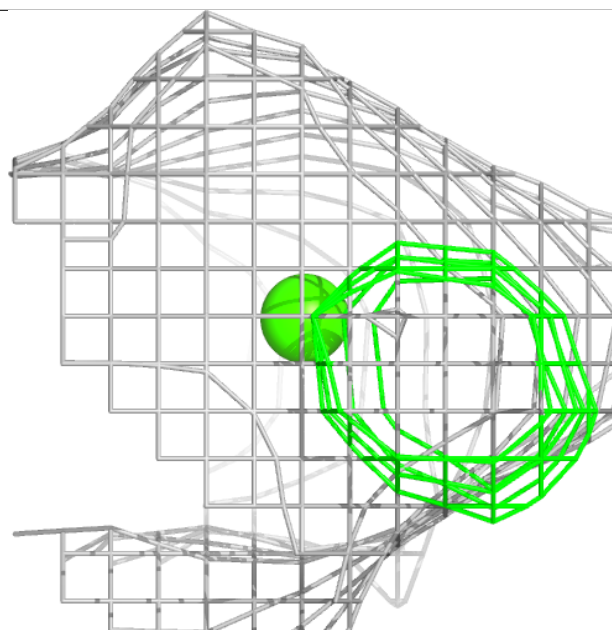
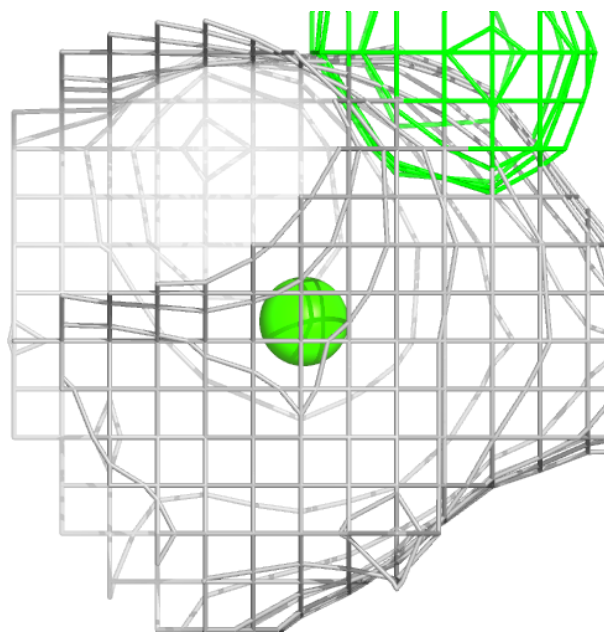
Electron density around ADP D 901:

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



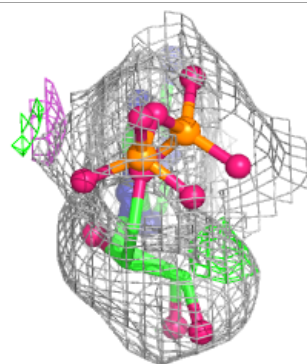
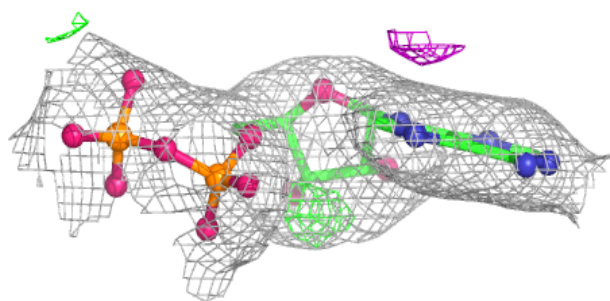
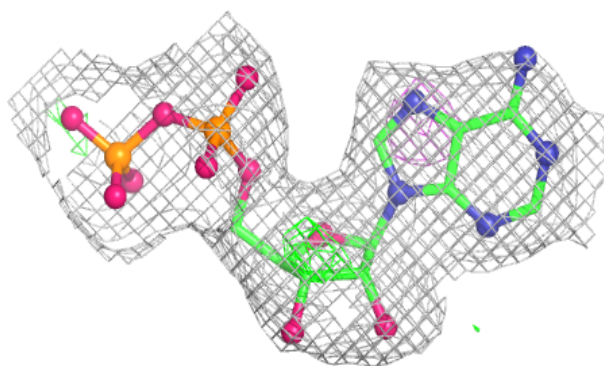
Electron density around CA B 902:

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

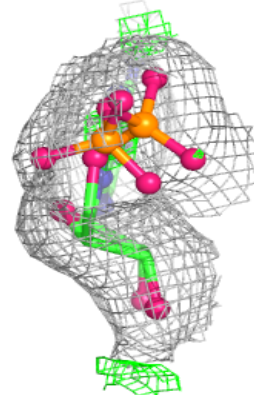
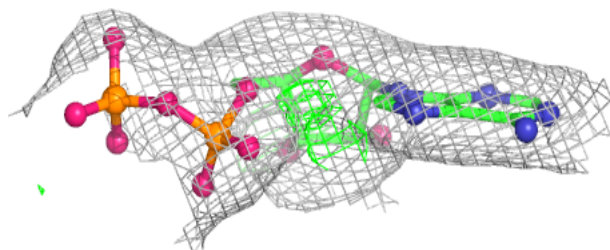
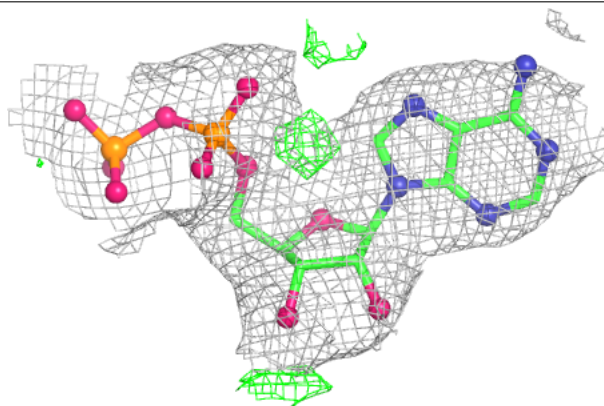


Electron density around ADP B 901:

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

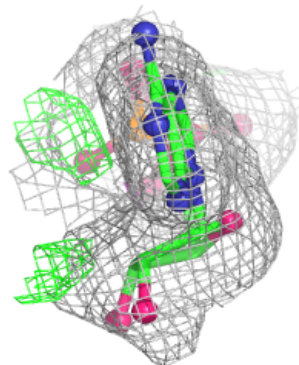
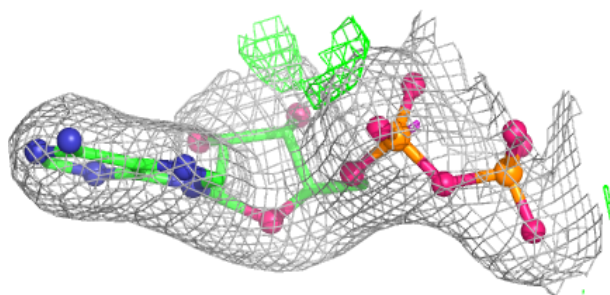
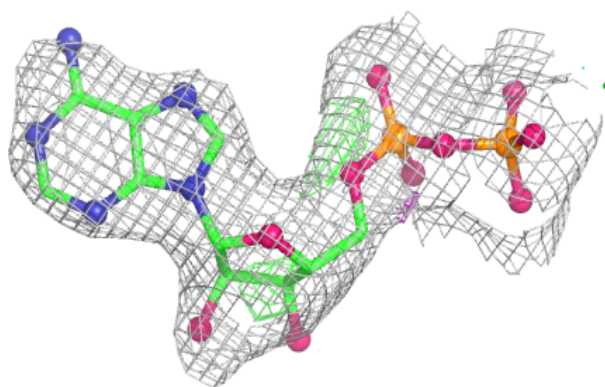
**Electron density around ADP A 901:**

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



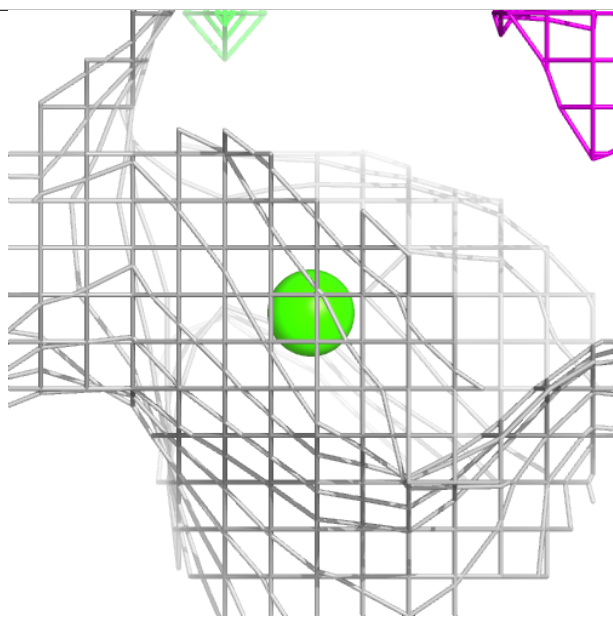
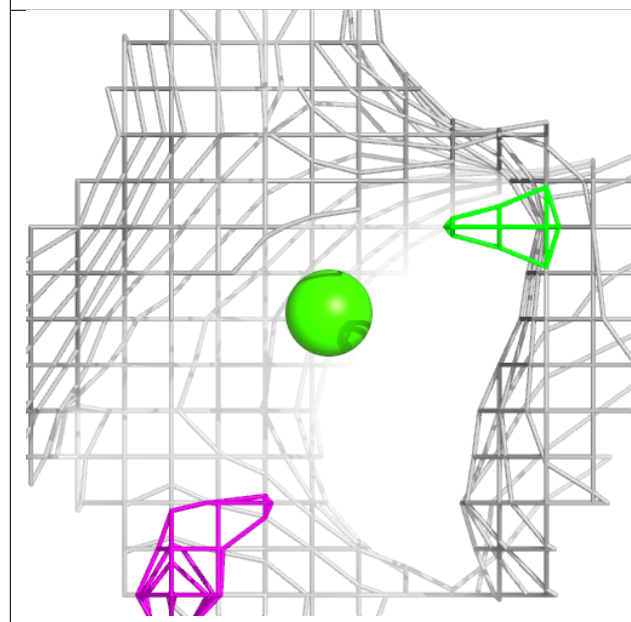
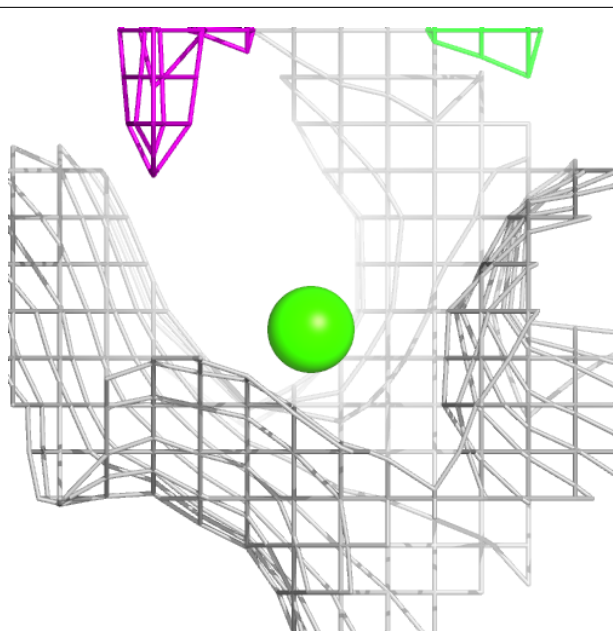
Electron density around ADP C 901:

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



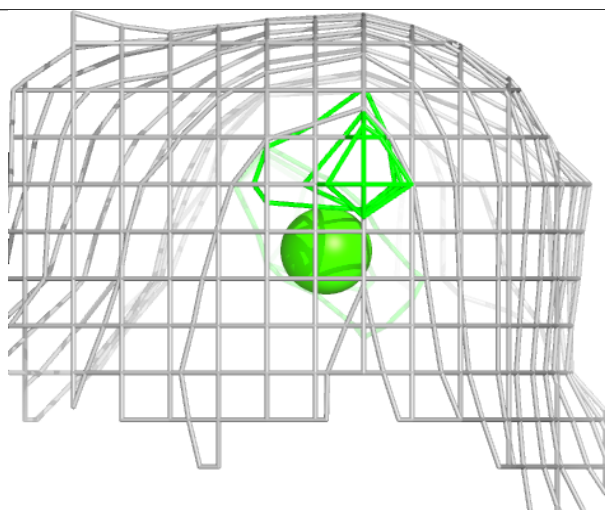
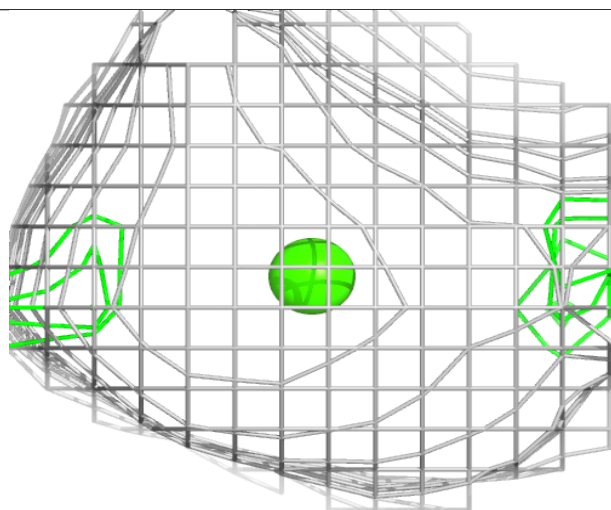
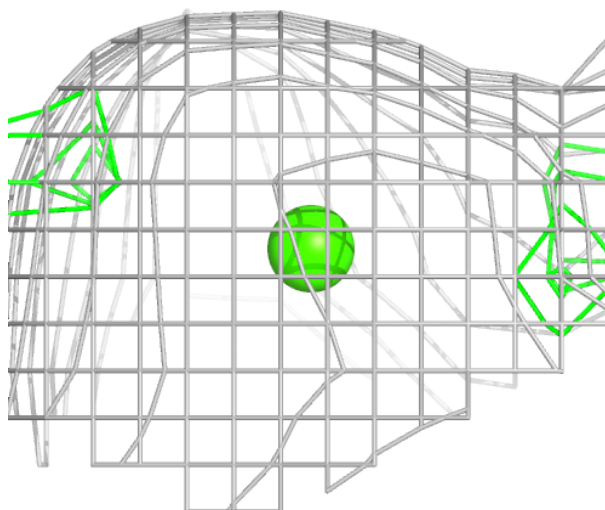
Electron density around CA D 902:

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



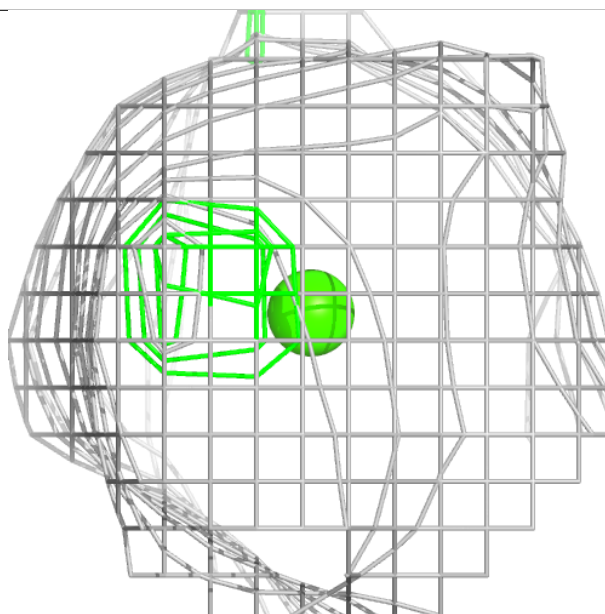
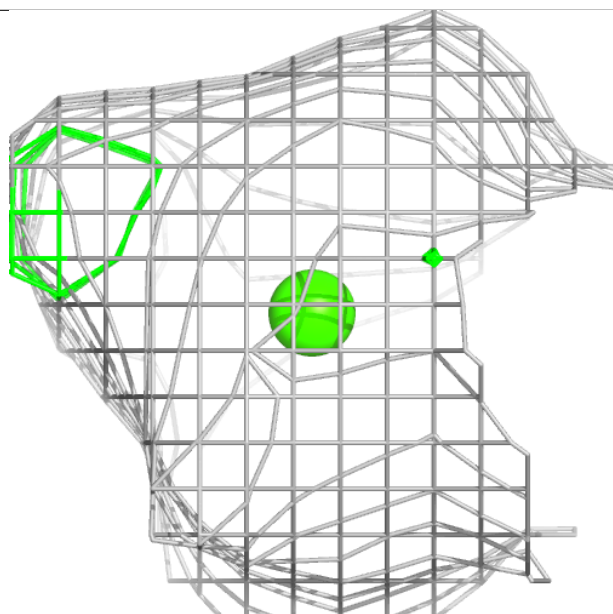
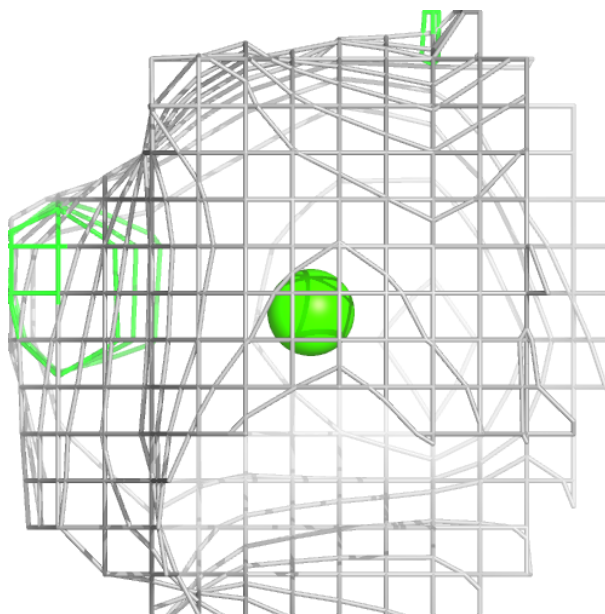
Electron density around CA A 902:

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



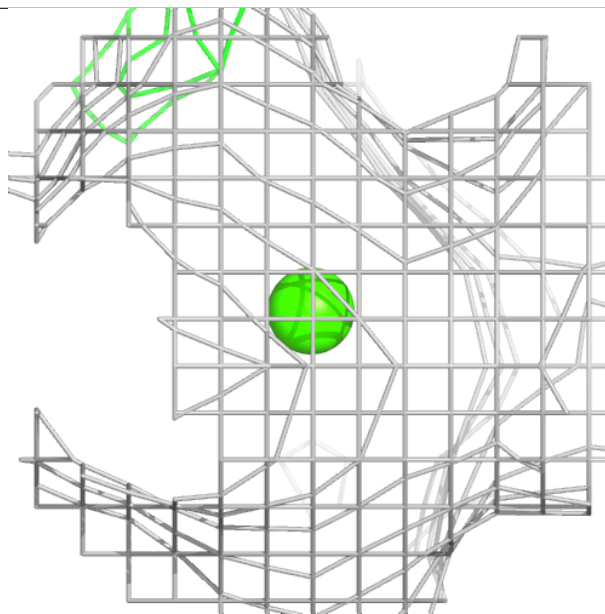
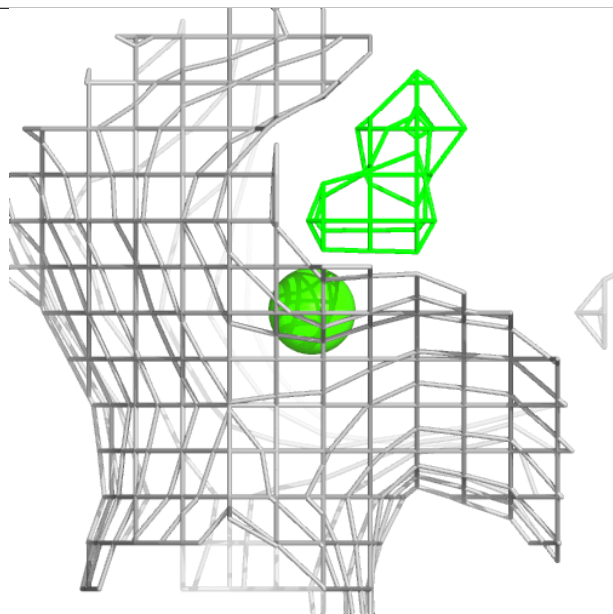
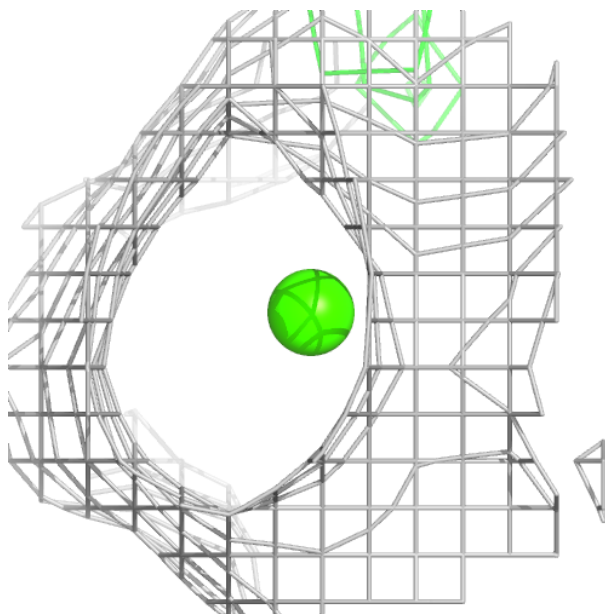
Electron density around CA C 902:

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



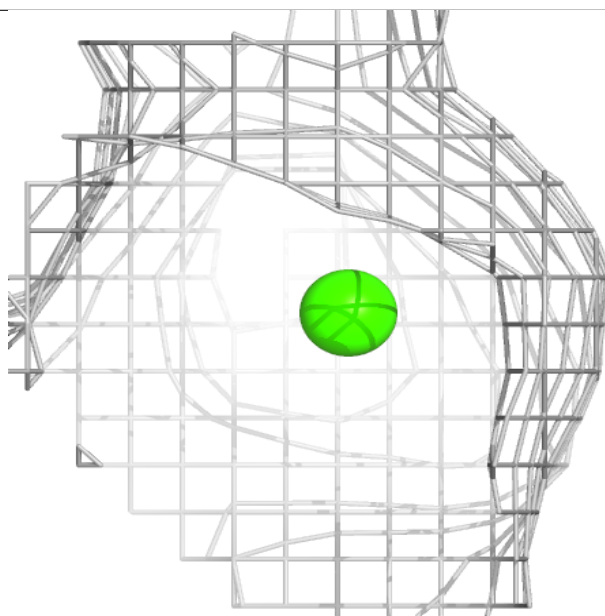
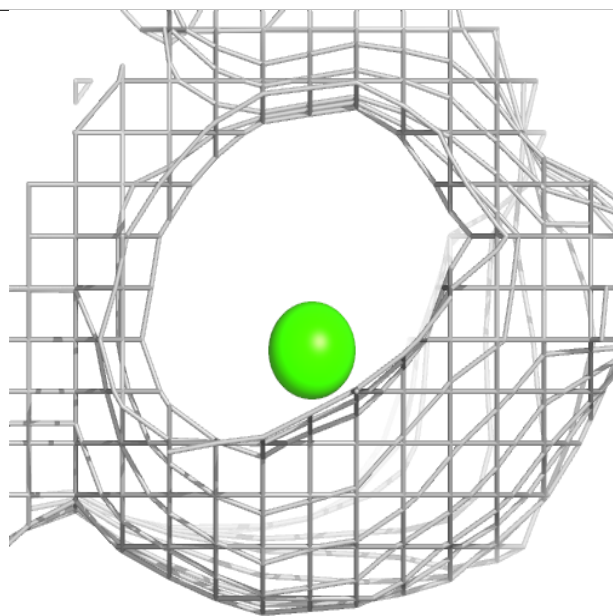
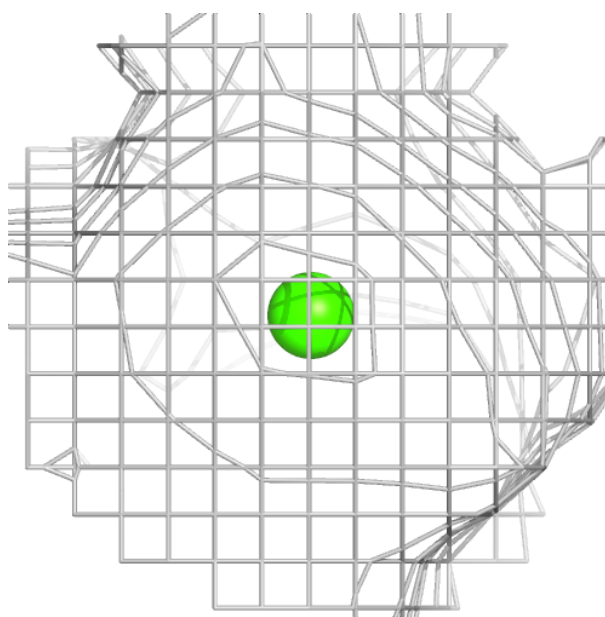
Electron density around CA A 903:

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



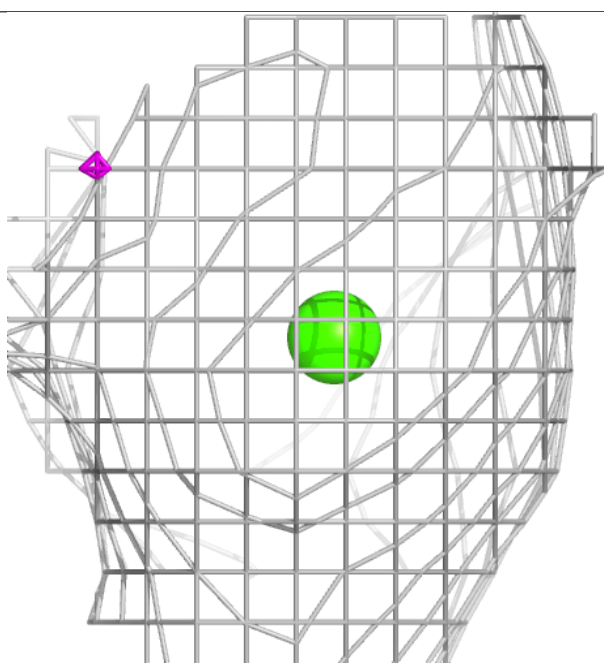
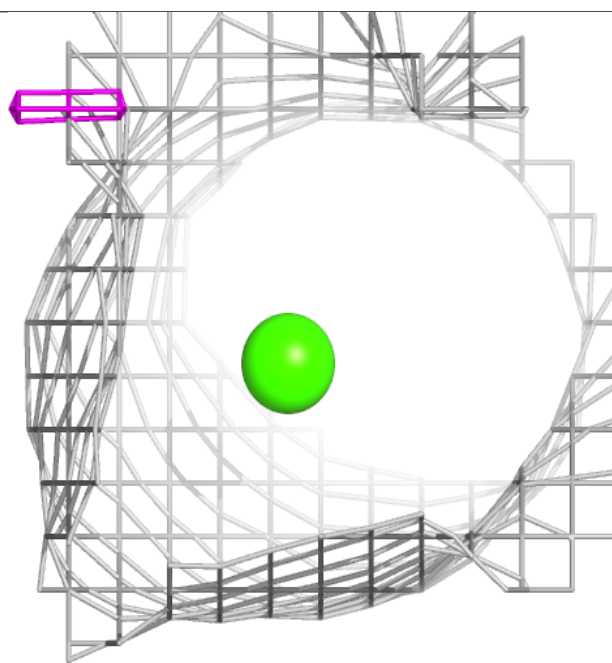
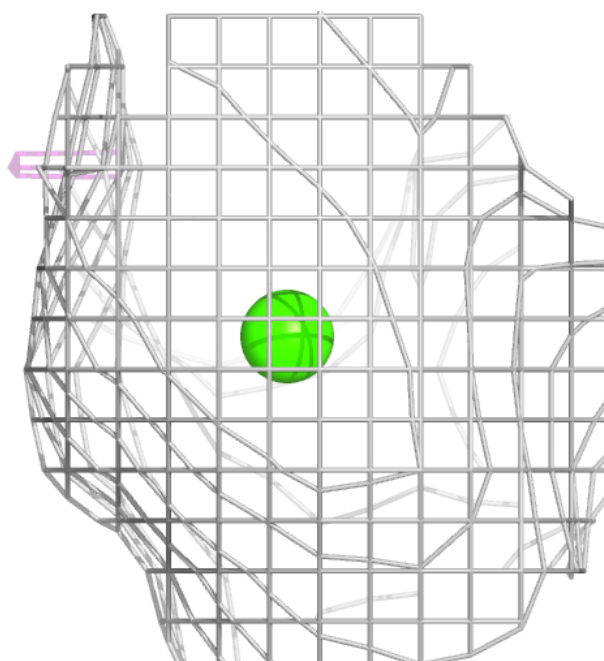
Electron density around CA B 903:

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



Electron density around CA C 903:

$2mF_o-DF_c$ (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.