



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2026 – 01:30 pm BST

PDB ID : 9TWB / pdb_00009twb
Title : Crystal structure of BRAF(val600):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 : 2026-01-14
Resolution : 2.45 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

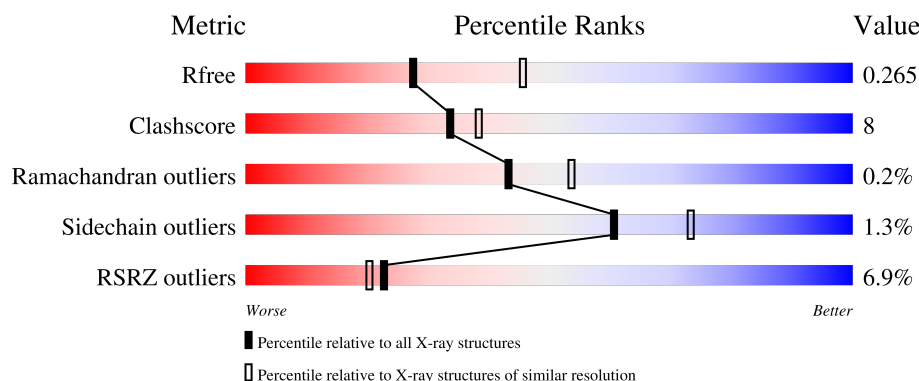
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	333	5% 66% 18% 16%
1	D	333	11% 65% 18% 16%
2	B	282	4% 78% 19% .
2	C	282	4% 79% 17% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8954 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	280	Total	C	N	O	P	S	0	0	0
			2202	1408	370	407	1	16			
1	D	279	Total	C	N	O	P	S	0	0	0
			2199	1409	369	404	1	16			

- 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	0	0
			2177	1377	385	402	13			
2	B	274	Total	C	N	O	S	0	0	0
			2201	1396	392	400	13			

There are 34 discrepancies between the modelled and reference sequences:

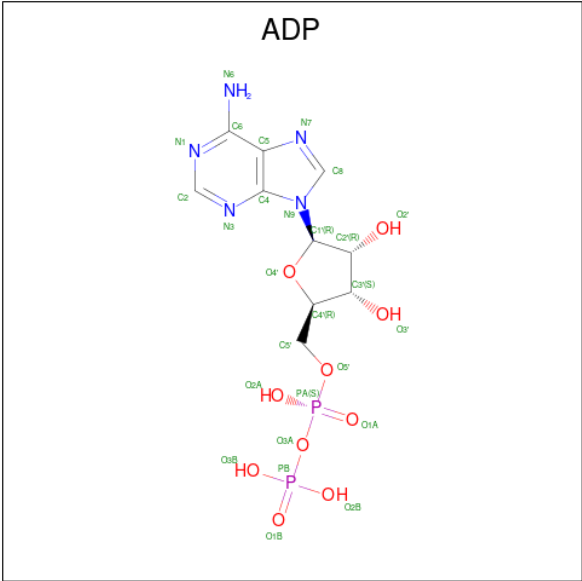
Chain	Residue	Modelled	Actual	Comment	Reference
C	442	SER	-	expression tag	UNP P15056
C	443	ASN	-	expression tag	UNP P15056
C	444	ALA	-	expression tag	UNP P15056
C	543	ALA	ILE	engineered mutation	UNP P15056
C	544	SER	ILE	engineered mutation	UNP P15056
C	551	LYS	ILE	engineered mutation	UNP P15056
C	562	ARG	GLN	engineered mutation	UNP P15056
C	588	ASN	LEU	engineered mutation	UNP P15056
C	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	engineered mutation	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
C	722	SER	PRO	engineered mutation	UNP P15056

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	723	GLY	LYS	engineered mutation	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	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	engineered mutation	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	PRO	engineered mutation	UNP P15056
B	723	GLY	LYS	engineered mutation	UNP P15056

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

Continued on next page...

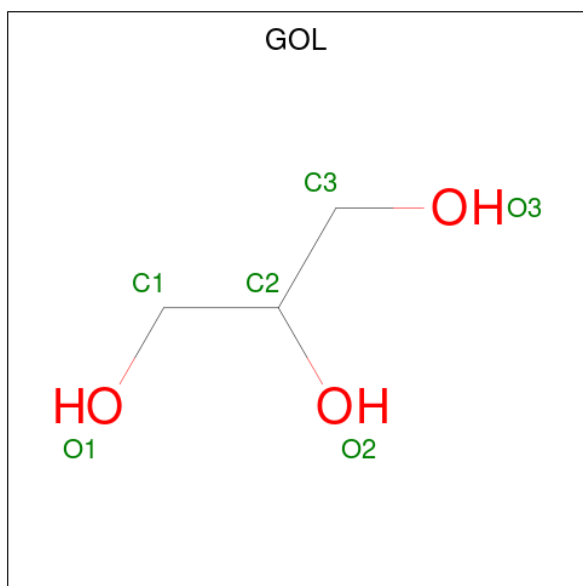
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	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).

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	C	1	Total	C	O	0	0
			6	3	3		
5	B	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

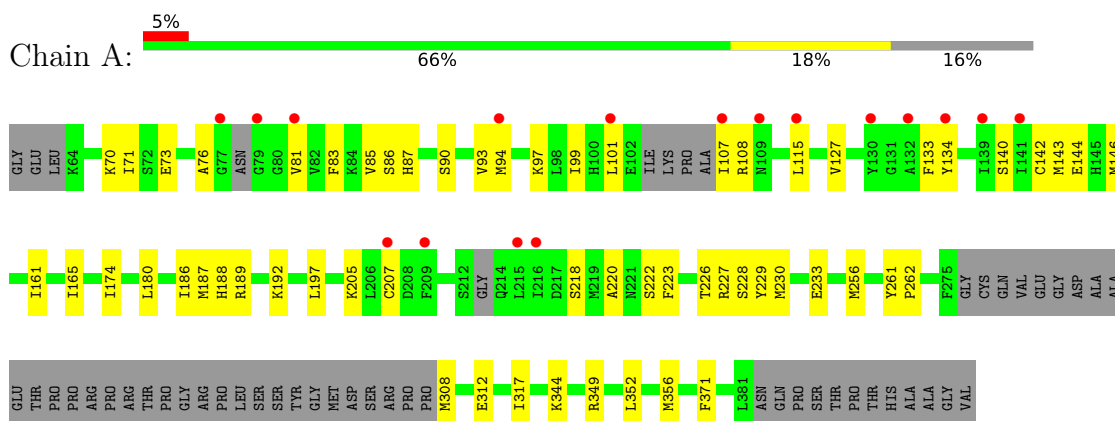
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total 13	O 13	0	0
7	C	15	Total 15	O 15	0	0
7	B	13	Total 13	O 13	0	0
7	D	5	Total 5	O 5	0	0

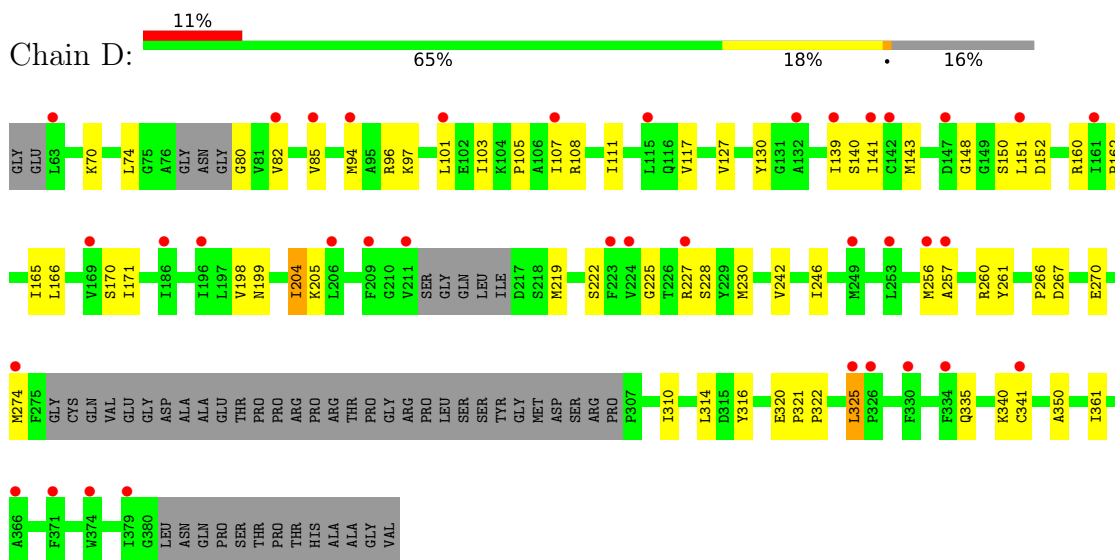
3 Residue-property plots [i](#)

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.

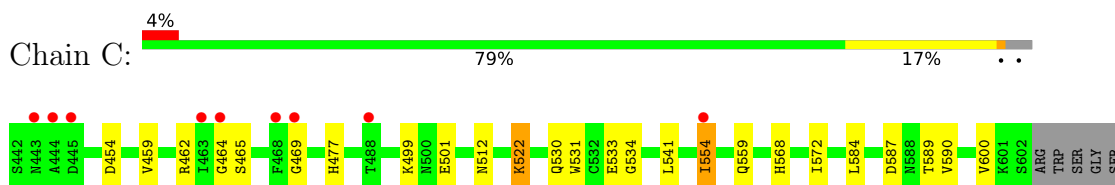
- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1



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

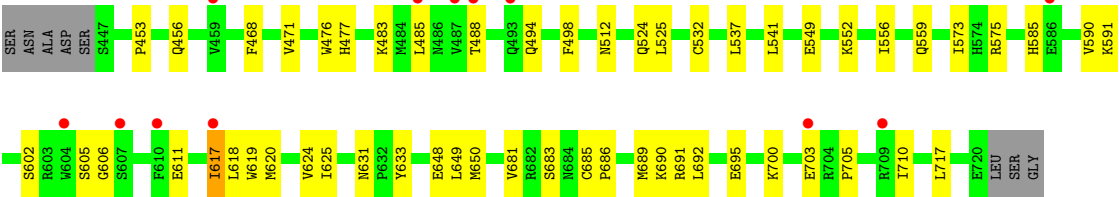
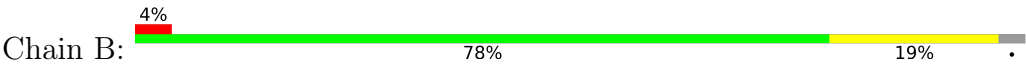


- Molecule 2: Serine/threonine-protein kinase B-raf





● 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	68.13Å 67.98Å 291.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.45 48.59 – 2.45	Depositor EDS
% Data completeness (in resolution range)	59.8 (48.59-2.45) 59.4 (48.59-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.45Å)	Xtriage
Refinement program	PHENIX v1.20	Depositor
R, R_{free}	0.219 , 0.265 0.219 , 0.265	Depositor DCC
R_{free} test set	2001 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8954	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, SEP, NA, 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	0.12	0/2233	0.29	0/3002
1	D	0.11	0/2233	0.28	1/3005 (0.0%)
2	B	0.10	0/2250	0.27	0/3033
2	C	0.11	0/2221	0.27	0/2993
All	All	0.11	0/8937	0.28	1/12033 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	117	VAL	N-CA-C	-5.63	105.94	112.98

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	683	SER	Peptide

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	2202	0	2217	38	0
1	D	2199	0	2221	39	0
2	B	2201	0	2204	31	0
2	C	2177	0	2184	33	0
3	A	27	0	12	3	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	3	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	B	6	0	8	0	0
5	C	6	0	8	2	0
6	B	1	0	0	0	0
7	A	13	0	0	0	0
7	B	13	0	0	0	0
7	C	15	0	0	2	0
7	D	5	0	0	0	0
All	All	8954	0	8890	137	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 8.

All (137) 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:D:171:ILE:HG12	1:D:361:ILE:HG23	1.66	0.78
2:C:617:ILE:HA	2:C:620:MET:HE2	1.70	0.72
2:B:602:SER:H	2:B:605:SER:HB2	1.53	0.72
2:C:587:ASP:HB3	2:C:589:THR:HG22	1.73	0.71
1:A:133:PHE:HB3	1:A:140:SER:HB3	1.72	0.70
1:A:97:LYS:HG2	1:A:99:ILE:HD11	1.74	0.69
2:B:686:PRO:HG2	2:B:717:LEU:HD11	1.75	0.69
2:C:559:GLN:NE2	7:C:1002:HOH:O	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:MET:HE2	1:A:312:GLU:HB3	1.80	0.63
1:A:317:ILE:O	1:A:344:LYS:NZ	2.29	0.63
1:A:228:SER:O	1:A:261:TYR:OH	2.17	0.62
2:B:471:VAL:HG22	2:B:483:LYS:HG2	1.83	0.61
1:D:143:MET:HE2	3:D:901:ADP:HN61	1.66	0.60
1:A:146:MET:HG3	1:A:197:LEU:HD23	1.82	0.60
2:C:651:THR:HG22	2:C:681:VAL:HA	1.82	0.60
1:D:246:ILE:HG22	1:D:341:CYS:HB2	1.84	0.60
2:B:681:VAL:HG21	2:B:690:LYS:HD2	1.84	0.59
2:C:688:ARG:HD3	2:C:713:GLU:HG3	1.85	0.59
2:C:692:LEU:HD21	2:C:710:ILE:HG23	1.84	0.59
1:D:340:LYS:HG2	1:D:350:ALA:HB2	1.84	0.58
1:D:198:VAL:HG12	1:D:204:ILE:HG22	1.85	0.57
1:D:228:SER:O	1:D:261:TYR:OH	2.19	0.57
2:B:620:MET:HE2	2:B:625:ILE:HG12	1.85	0.57
1:A:71:ILE:HD11	1:A:86:SER:HB2	1.85	0.57
1:A:174:ILE:HG23	1:A:352:LEU:HD12	1.87	0.57
2:C:665:ILE:HD12	1:D:219:MET:HG2	1.85	0.57
2:B:541:LEU:HD11	2:B:649:LEU:HD23	1.86	0.57
2:B:619:TRP:NE1	2:B:648:GLU:OE2	2.37	0.57
1:A:161:ILE:HD12	1:A:256:MET:HB3	1.88	0.56
2:C:554:ILE:HG12	2:C:717:LEU:HD12	1.87	0.56
1:D:148:GLY:H	1:D:199:ASN:HA	1.70	0.56
1:A:197:LEU:HD21	3:A:901:ADP:C5	2.41	0.56
2:C:531:TRP:HE1	2:C:533:GLU:HG2	1.70	0.56
2:B:453:PRO:HG2	2:B:456:GLN:HG3	1.88	0.55
1:A:233:GLU:OE2	1:A:349:ARG:NH2	2.39	0.55
1:D:70:LYS:HA	1:D:85:VAL:HG12	1.87	0.55
2:B:650:MET:HE3	2:B:689:MET:HG2	1.90	0.54
3:C:901:ADP:O1A	5:C:904:GOL:O2	2.24	0.54
2:C:620:MET:HE3	2:C:625:ILE:HG12	1.89	0.54
1:A:174:ILE:HG22	1:A:356:MET:HE2	1.91	0.53
2:B:692:LEU:HD21	2:B:710:ILE:HG23	1.90	0.53
1:D:260:ARG:HD2	1:D:274:MET:HE1	1.91	0.53
1:D:227:ARG:HD2	1:D:261:TYR:CG	2.44	0.53
1:A:144:GLU:OE2	1:A:205:LYS:NZ	2.36	0.52
2:C:454:ASP:HB3	2:C:522:LYS:HG3	1.92	0.52
2:C:501:GLU:OE2	5:C:904:GOL:O1	2.22	0.52
1:D:148:GLY:HA3	1:D:198:VAL:HG23	1.92	0.52
1:D:74:LEU:HB2	1:D:82:VAL:HG12	1.92	0.51
1:A:144:GLU:O	3:A:901:ADP:N6	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD22	1:A:207:CYS:SG	2.51	0.51
2:C:462:ARG:NH2	2:C:465:SER:O	2.43	0.51
2:C:705:PRO:HG2	2:C:710:ILE:HD11	1.93	0.51
1:D:105:PRO:HA	1:D:108:ARG:HD3	1.93	0.50
1:D:151:LEU:HD23	1:D:256:MET:HE1	1.94	0.50
1:D:325:LEU:HD23	1:D:335:GLN:HG2	1.92	0.50
1:D:96:ARG:HE	1:D:140:SER:HB3	1.76	0.50
1:D:127:VAL:HA	1:D:205:LYS:HD3	1.92	0.50
2:C:541:LEU:HD11	2:C:649:LEU:HD23	1.95	0.49
2:C:636:GLN:HG2	2:C:701:ARG:O	2.12	0.49
2:C:617:ILE:HD11	1:D:219:MET:HG3	1.95	0.49
1:A:94:MET:HE3	1:A:142:CYS:HB3	1.95	0.49
1:D:162:PRO:HD2	1:D:165:ILE:HD12	1.93	0.49
2:C:616:SER:O	2:C:620:MET:HG3	2.13	0.48
2:B:549:GLU:HG2	2:B:552:LYS:HB2	1.95	0.48
1:D:80:GLY:N	3:D:901:ADP:O2B	2.46	0.48
2:B:611:GLU:N	2:B:611:GLU:OE1	2.46	0.48
2:B:620:MET:HE3	2:B:624:VAL:HG12	1.96	0.48
1:D:97:LYS:NZ	3:D:901:ADP:O1A	2.45	0.48
1:A:76:ALA:HB2	1:A:81:VAL:HG13	1.96	0.47
1:D:230:MET:HE2	1:D:230:MET:HB2	1.75	0.47
1:A:97:LYS:HE2	1:A:99:ILE:HD11	1.97	0.47
1:A:188:HIS:NE2	1:A:207:CYS:O	2.47	0.47
2:C:658:ASN:OD1	2:C:658:ASN:N	2.45	0.47
2:B:532:CYS:SG	2:B:585:HIS:HB2	2.54	0.47
2:B:606:GLY:HA2	2:B:631:ASN:ND2	2.29	0.47
1:A:187:MET:HE2	1:A:189:ARG:HG2	1.97	0.47
1:A:218:SER:C	1:A:220:ALA:H	2.23	0.47
1:A:108:ARG:HG3	1:A:134:TYR:HE2	1.80	0.47
2:B:537:LEU:HD21	2:B:649:LEU:HD21	1.97	0.47
1:A:87:HIS:HD2	1:A:90:SER:HB3	1.79	0.47
1:D:267:ASP:OD1	1:D:270:GLU:HB2	2.15	0.46
2:C:464:GLY:HA3	2:C:469:GLY:HA3	1.96	0.46
1:D:94:MET:HE2	1:D:130:TYR:HD2	1.80	0.46
1:D:260:ARG:HD3	1:D:266:PRO:HG3	1.96	0.46
2:B:485:LEU:HD11	2:B:498:PHE:HB2	1.97	0.46
2:C:617:ILE:HD13	2:C:662:ARG:HG3	1.98	0.45
2:C:477:HIS:CE1	2:B:591:LYS:HE3	2.51	0.45
2:B:618:LEU:HB2	2:B:619:TRP:CE3	2.52	0.45
1:D:150:SER:OG	1:D:152:ASP:OD1	2.29	0.45
1:D:204:ILE:O	1:D:205:LYS:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:ILE:HG22	2:B:575:ARG:HG2	1.99	0.44
2:B:575:ARG:HD2	2:B:633:TYR:CG	2.52	0.44
1:D:160:ARG:HD3	1:D:257:ALA:O	2.17	0.44
1:A:226:THR:OG1	1:A:227:ARG:N	2.48	0.44
2:C:512:ASN:HA	2:C:590:VAL:O	2.18	0.44
1:D:321:PRO:HA	1:D:322:PRO:HD3	1.89	0.44
1:A:127:VAL:HA	1:A:205:LYS:HD3	2.00	0.44
1:D:166:LEU:O	1:D:170:SER:OG	2.26	0.43
1:A:70:LYS:HA	1:A:85:VAL:HG12	1.99	0.43
1:D:316:TYR:O	1:D:320:GLU:HB2	2.18	0.43
2:B:556:ILE:HG23	2:B:590:VAL:HG11	2.00	0.43
2:B:700:LYS:NZ	2:B:703:GLU:HG3	2.34	0.43
2:C:512:ASN:ND2	2:C:559:GLN:HB3	2.34	0.43
1:A:107:ILE:HG12	1:A:108:ARG:H	1.84	0.42
1:A:165:ILE:HG23	1:A:371:PHE:CE2	2.54	0.42
1:A:101:LEU:HD22	1:A:134:TYR:HE1	1.85	0.42
2:B:524:GLN:HG2	2:B:525:LEU:H	1.84	0.42
1:A:192:LYS:HE2	1:A:229:TYR:CD1	2.55	0.42
1:D:97:LYS:HB3	1:D:141:ILE:HB	2.01	0.42
2:C:530:GLN:HE22	2:B:477:HIS:HB3	1.83	0.42
2:B:468:PHE:CD2	2:B:494:GLN:HG3	2.55	0.42
1:D:107:ILE:O	1:D:111:ILE:HG13	2.20	0.42
2:C:454:ASP:OD1	2:C:454:ASP:N	2.45	0.41
2:C:572:ILE:HG12	2:C:600:VAL:HG22	2.02	0.41
1:A:180:LEU:HB3	1:A:186:ILE:HG23	2.02	0.41
2:C:534:GLY:HA3	2:C:584:LEU:O	2.20	0.41
1:D:242:VAL:O	1:D:246:ILE:HG13	2.21	0.41
1:A:143:MET:HG3	3:A:901:ADP:HN61	1.85	0.41
1:A:261:TYR:HA	1:A:262:PRO:HD3	1.92	0.41
1:D:151:LEU:HD12	1:D:151:LEU:HA	1.83	0.41
2:B:705:PRO:HG2	2:B:710:ILE:HD11	2.03	0.41
2:C:626:ARG:HB3	2:C:628:GLN:HG3	2.03	0.41
2:B:456:GLN:HB3	2:B:476:TRP:HE1	1.85	0.41
2:B:512:ASN:ND2	2:B:559:GLN:HB3	2.35	0.41
1:D:101:LEU:HD22	1:D:139:ILE:CG1	2.51	0.41
1:A:107:ILE:HG12	1:A:108:ARG:N	2.36	0.41
1:A:223:PHE:CE1	2:B:617:ILE:HG23	2.56	0.41
1:A:146:MET:HG3	1:A:197:LEU:HB3	2.02	0.41
2:C:686:PRO:HG2	2:C:717:LEU:HD11	2.03	0.40
2:C:499:LYS:NZ	7:C:1007:HOH:O	2.54	0.40
2:B:691:ARG:O	2:B:695:GLU:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:PRO:O	1:D:166:LEU:HD23	2.20	0.40
1:A:73:GLU:HG2	1:A:83:PHE:CD2	2.57	0.40
1:A:233:GLU:CD	1:A:349:ARG:HH22	2.28	0.40
2:C:568:HIS:CG	2:C:635:PHE:HD2	2.39	0.40
2:C:639:VAL:HG12	2:C:707:PHE:CE2	2.56	0.40
1:D:310:ILE:O	1:D:314:LEU:HG	2.21	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	269/333 (81%)	256 (95%)	13 (5%)	0	100	100
1	D	270/333 (81%)	256 (95%)	13 (5%)	1 (0%)	30	37
2	B	272/282 (96%)	264 (97%)	7 (3%)	1 (0%)	30	37
2	C	269/282 (95%)	252 (94%)	17 (6%)	0	100	100
All	All	1080/1230 (88%)	1028 (95%)	50 (5%)	2 (0%)	43	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	225	GLY
2	B	685	CYS

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	243/284 (86%)	240 (99%)	3 (1%)	63	74
1	D	243/284 (86%)	240 (99%)	3 (1%)	63	74
2	B	241/247 (98%)	239 (99%)	2 (1%)	73	83
2	C	240/247 (97%)	235 (98%)	5 (2%)	47	62
All	All	967/1062 (91%)	954 (99%)	13 (1%)	61	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	A	115	LEU
1	A	230	MET
2	C	459	VAL
2	C	522	LYS
2	C	554	ILE
2	C	624	VAL
2	C	639	VAL
2	B	488	THR
2	B	617	ILE
1	D	103	ILE
1	D	204	ILE
1	D	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
2	C	496	GLN
2	C	530	GLN
2	B	500	ASN
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	1.56	1 (12%)	8,12,14	1.56	2 (25%)
1	SEP	D	222	1	8,9,10	1.48	1 (12%)	8,12,14	1.40	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	-	4/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	SEP	P-O1P	3.40	1.61	1.50
1	D	222	SEP	P-O1P	3.26	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	SEP	P-OG-CB	-2.98	110.09	118.30
1	A	222	SEP	OG-CB-CA	2.68	110.75	108.14
1	D	222	SEP	P-OG-CB	-2.60	111.14	118.30
1	D	222	SEP	OG-CB-CA	2.16	110.25	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	222	SEP	N-CA-CB-OG
1	D	222	SEP	CB-OG-P-O2P
1	D	222	SEP	CB-OG-P-O1P
1	D	222	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
3	ADP	C	901	4	27,29,29	1.36	4 (14%)	42,45,45	1.94	11 (26%)
3	ADP	B	901	4	27,29,29	1.36	4 (14%)	42,45,45	1.89	10 (23%)
3	ADP	D	901	4	27,29,29	1.36	4 (14%)	42,45,45	1.93	11 (26%)
5	GOL	C	904	-	5,5,5	0.89	0	5,5,5	1.02	0
5	GOL	B	905	-	5,5,5	0.81	0	5,5,5	1.08	0
3	ADP	A	901	4	27,29,29	1.36	4 (14%)	42,45,45	1.94	11 (26%)

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
3	ADP	C	901	4	-	3/16/32/32	0/3/3/3
3	ADP	B	901	4	-	5/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	901	4	-	2/16/32/32	0/3/3/3
5	GOL	C	904	-	-	2/4/4/4	-
5	GOL	B	905	-	-	2/4/4/4	-
3	ADP	A	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	C	901	ADP	C5-C4	4.55	1.47	1.39
3	D	901	ADP	C5-C4	4.54	1.47	1.39
3	B	901	ADP	C5-C4	4.54	1.47	1.39
3	A	901	ADP	C5-C4	4.49	1.47	1.39
3	A	901	ADP	C5-C6	2.77	1.48	1.41
3	C	901	ADP	C5-C6	2.73	1.48	1.41
3	D	901	ADP	C5-C6	2.71	1.48	1.41
3	B	901	ADP	C5-C6	2.65	1.48	1.41
3	B	901	ADP	C8-N7	2.47	1.36	1.31
3	D	901	ADP	C8-N7	2.45	1.36	1.31
3	C	901	ADP	C8-N7	2.45	1.36	1.31
3	A	901	ADP	C8-N7	2.41	1.36	1.31
3	A	901	ADP	C5-N7	-2.17	1.34	1.39
3	B	901	ADP	C5-N7	-2.14	1.35	1.39
3	C	901	ADP	C5-N7	-2.12	1.35	1.39
3	D	901	ADP	C5-N7	-2.10	1.35	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ADP	C5-C4-N3	-6.32	118.50	126.75
3	C	901	ADP	C5-C4-N3	-6.20	118.66	126.75
3	D	901	ADP	C5-C4-N3	-6.06	118.84	126.75
3	B	901	ADP	C5-C4-N3	-6.05	118.86	126.75
3	A	901	ADP	N3-C4-N9	4.90	135.16	127.08
3	C	901	ADP	N3-C4-N9	4.81	135.00	127.08
3	B	901	ADP	N3-C4-N9	4.73	134.87	127.08
3	D	901	ADP	N3-C4-N9	4.69	134.81	127.08
3	C	901	ADP	C2-N3-C4	3.87	120.90	111.75
3	A	901	ADP	C2-N3-C4	3.87	120.89	111.75
3	B	901	ADP	C2-N3-C4	3.82	120.77	111.75
3	D	901	ADP	C2-N3-C4	3.81	120.75	111.75
3	A	901	ADP	C4-C5-N7	-3.40	106.48	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ADP	C4-C5-N7	-3.34	106.55	110.62
3	C	901	ADP	C4-C5-N7	-3.29	106.61	110.62
3	B	901	ADP	C4-C5-N7	-3.17	106.76	110.62
3	B	901	ADP	N3-C2-N1	-3.17	123.64	128.60
3	C	901	ADP	N3-C2-N1	-3.11	123.74	128.60
3	D	901	ADP	N3-C2-N1	-3.09	123.77	128.60
3	A	901	ADP	N3-C2-N1	-3.01	123.90	128.60
3	A	901	ADP	C5-N7-C8	2.91	107.65	103.51
3	D	901	ADP	PA-O3A-PB	-2.81	123.18	132.83
3	D	901	ADP	C5-N7-C8	2.79	107.47	103.51
3	C	901	ADP	C5-N7-C8	2.76	107.43	103.51
3	B	901	ADP	C5-N7-C8	2.65	107.28	103.51
3	A	901	ADP	PA-O3A-PB	-2.65	123.72	132.83
3	C	901	ADP	PA-O3A-PB	-2.63	123.80	132.83
3	D	901	ADP	C4-N9-C8	2.61	108.56	105.73
3	A	901	ADP	C4-N9-C8	2.60	108.55	105.73
3	B	901	ADP	C4-N9-C8	2.56	108.50	105.73
3	C	901	ADP	C3'-C2'-C1'	2.53	106.24	101.43
3	C	901	ADP	C4-N9-C8	2.51	108.44	105.73
3	B	901	ADP	C3'-C2'-C1'	2.34	105.88	101.43
3	D	901	ADP	C3'-C2'-C1'	2.32	105.83	101.43
3	D	901	ADP	C6-C5-N7	2.27	136.26	132.02
3	B	901	ADP	PA-O3A-PB	-2.20	125.26	132.83
3	C	901	ADP	C6-C5-N7	2.20	136.12	132.02
3	A	901	ADP	C6-C5-N7	2.17	136.06	132.02
3	B	901	ADP	C6-C5-N7	2.16	136.05	132.02
3	A	901	ADP	C3'-C2'-C1'	2.15	105.51	101.43
3	A	901	ADP	N9-C8-N7	-2.14	110.98	113.91
3	D	901	ADP	N9-C8-N7	-2.08	111.07	113.91
3	C	901	ADP	N9-C8-N7	-2.00	111.17	113.91

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	901	ADP	C5'-O5'-PA-O2A
3	B	901	ADP	O4'-C4'-C5'-O5'
3	C	901	ADP	O4'-C4'-C5'-O5'
3	B	901	ADP	C3'-C4'-C5'-O5'
3	D	901	ADP	O4'-C4'-C5'-O5'
5	B	905	GOL	O2-C2-C3-O3
3	A	901	ADP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

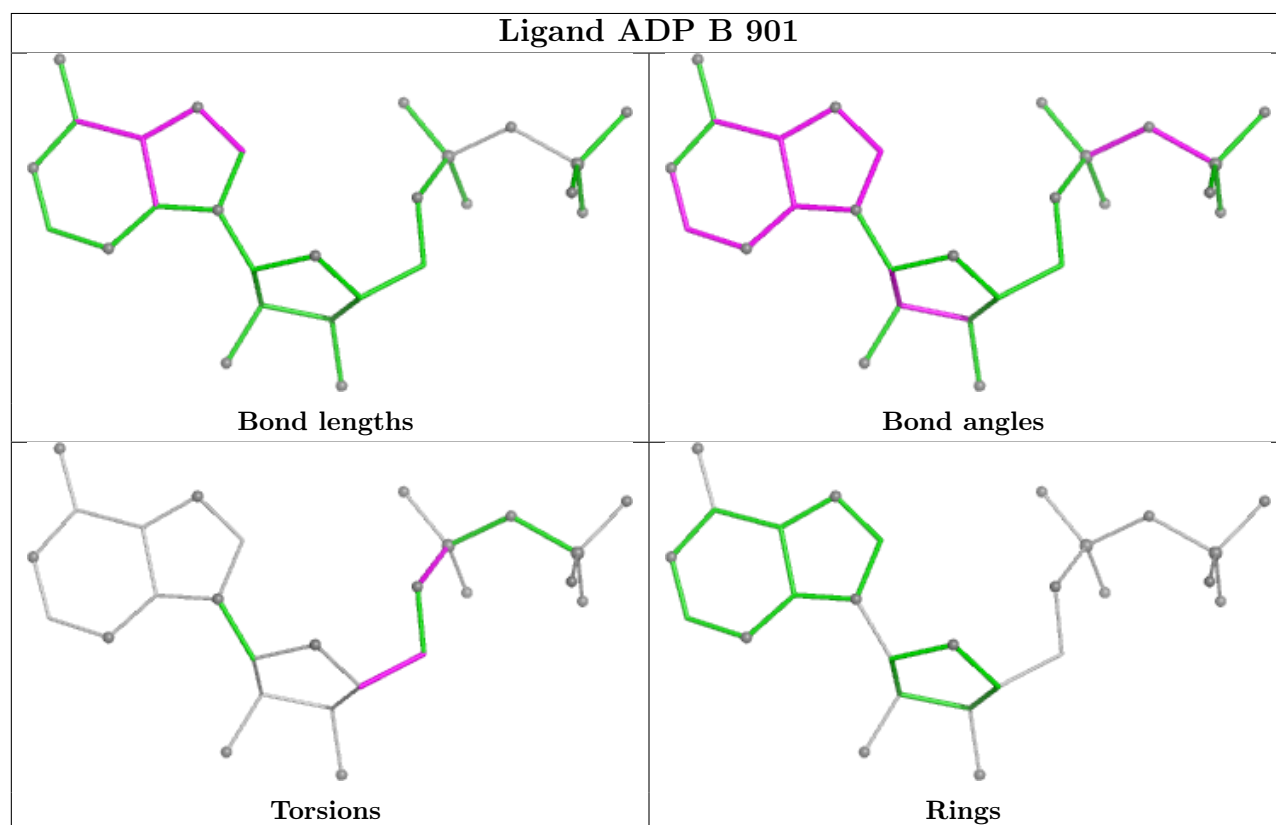
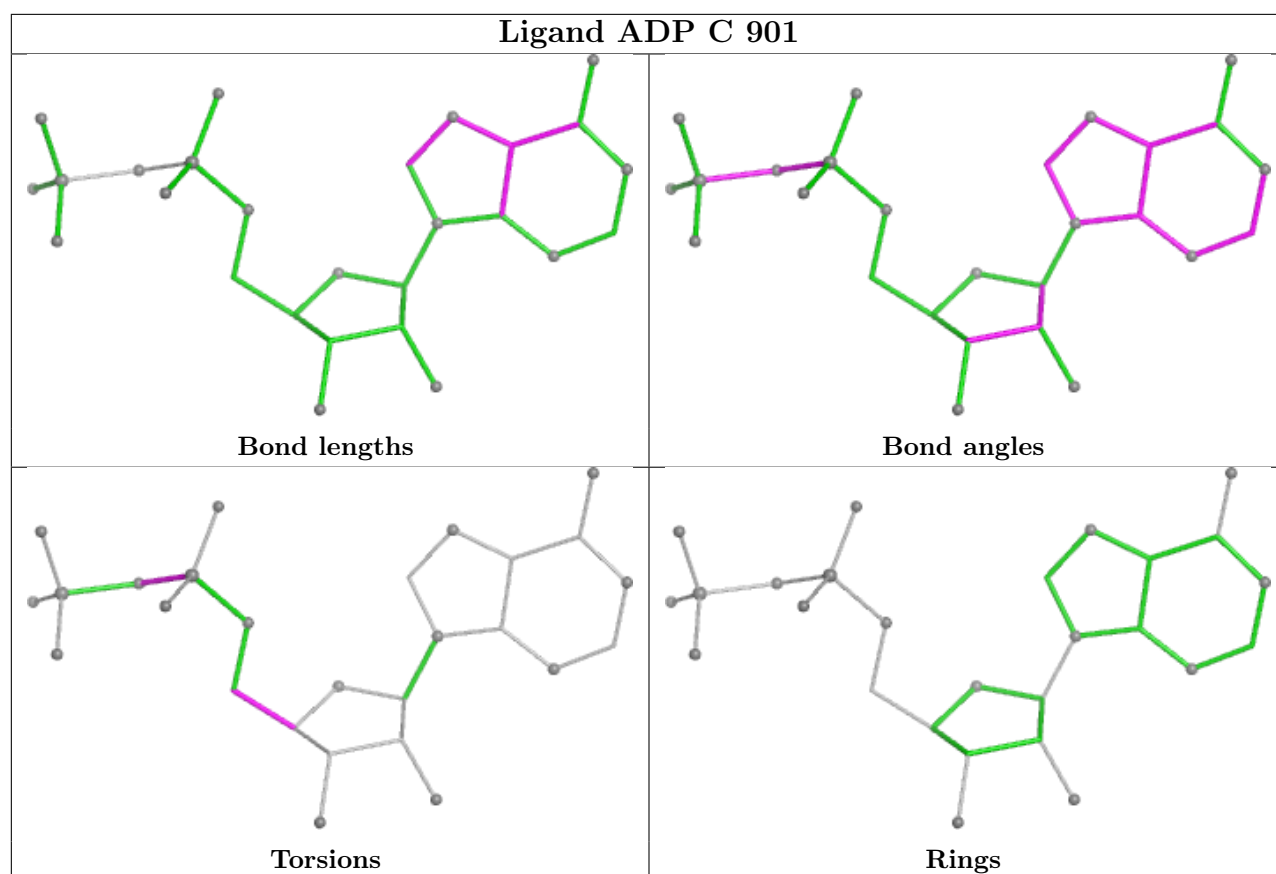
Mol	Chain	Res	Type	Atoms
3	C	901	ADP	C3'-C4'-C5'-O5'
3	D	901	ADP	C3'-C4'-C5'-O5'
5	C	904	GOL	O1-C1-C2-C3
5	B	905	GOL	C1-C2-C3-O3
3	A	901	ADP	C3'-C4'-C5'-O5'
5	C	904	GOL	O1-C1-C2-O2
3	A	901	ADP	PB-O3A-PA-O1A
3	B	901	ADP	C5'-O5'-PA-O3A
3	B	901	ADP	C5'-O5'-PA-O1A
3	A	901	ADP	PB-O3A-PA-O2A
3	C	901	ADP	PB-O3A-PA-O1A

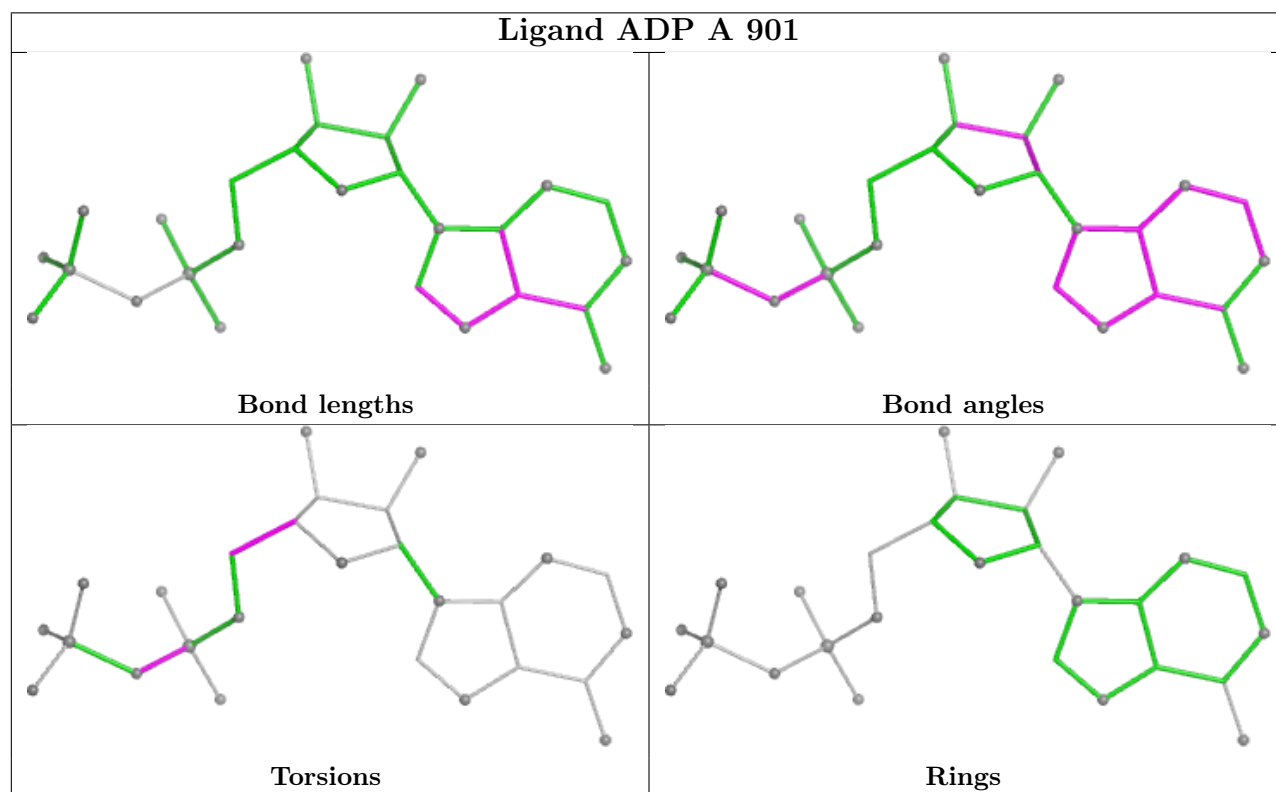
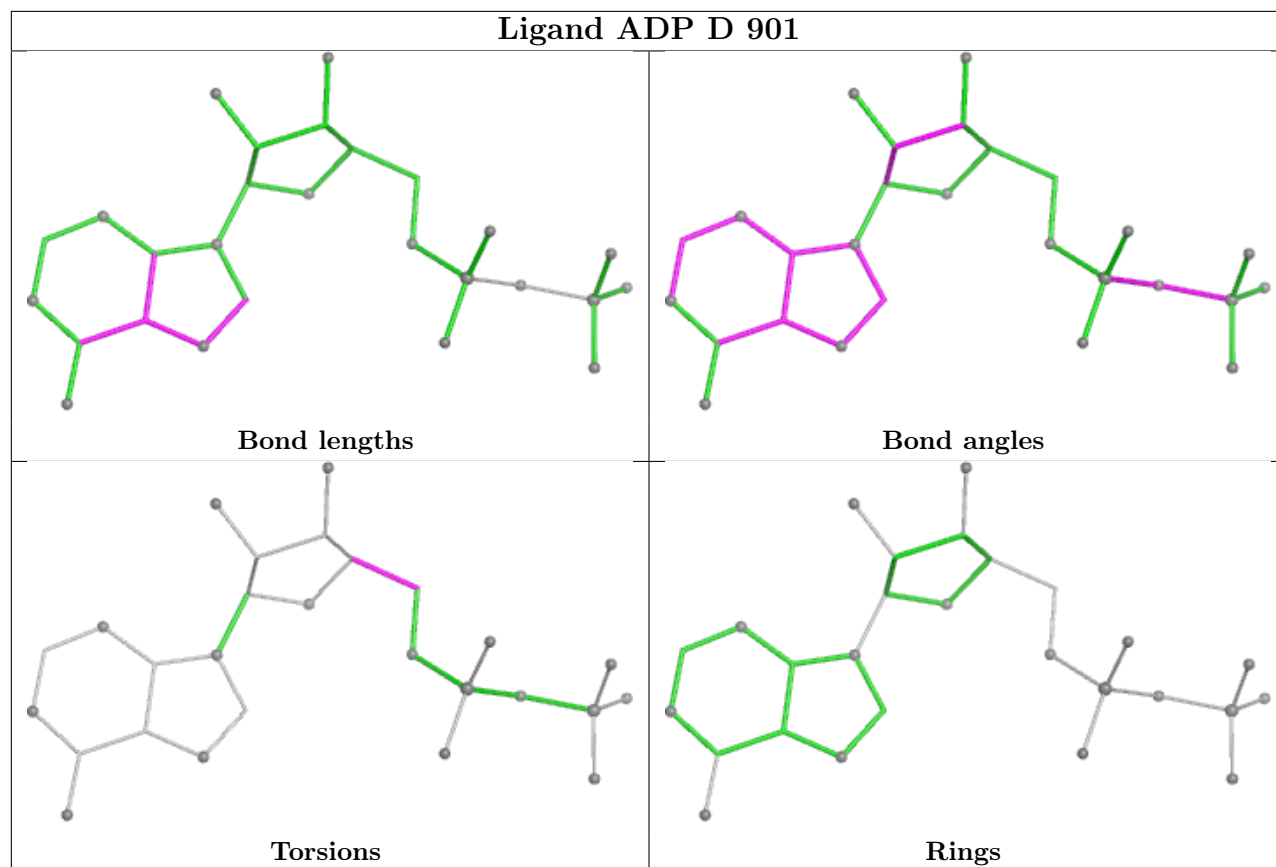
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	ADP	1	0
3	D	901	ADP	3	0
5	C	904	GOL	2	0
3	A	901	ADP	3	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, 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	279/333 (83%)	0.48	17 (6%) 27 24	48, 78, 169, 228	0
1	D	278/333 (83%)	0.83	37 (13%) 7 6	44, 114, 157, 210	0
2	B	274/282 (97%)	0.42	12 (4%) 39 38	38, 69, 142, 227	0
2	C	273/282 (96%)	0.32	10 (3%) 45 45	32, 68, 125, 201	0
All	All	1104/1230 (89%)	0.51	76 (6%) 23 20	32, 82, 154, 228	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ILE	6.3
1	A	215	LEU	4.9
1	D	326	PRO	4.4
1	D	223	PHE	4.3
1	D	186	ILE	4.2
1	D	101	LEU	4.0
1	A	107	ILE	3.9
1	D	142	CYS	3.8
1	D	253	LEU	3.6
1	D	169	VAL	3.5
1	D	132	ALA	3.4
1	D	334	PHE	3.4
2	B	604	TRP	3.3
1	D	224	VAL	3.2
2	B	617	ILE	3.2
1	D	330	PHE	3.2
1	A	209	PHE	3.1
1	D	211	VAL	3.1
2	C	443	ASN	3.0
2	C	464	GLY	2.8
1	D	115	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	256	MET	2.8
1	A	216	ILE	2.7
1	A	81	VAL	2.7
2	B	610	PHE	2.7
2	C	444	ALA	2.7
2	B	488	THR	2.7
1	A	134	TYR	2.7
2	C	717	LEU	2.7
1	A	141	ILE	2.6
1	D	139	ILE	2.6
1	A	132	ALA	2.6
1	A	79	GLY	2.6
1	A	94	MET	2.5
1	D	161	ILE	2.5
1	A	109	ASN	2.5
2	C	445	ASP	2.5
1	D	63	LEU	2.5
1	D	209	PHE	2.4
2	B	703	GLU	2.4
1	A	207	CYS	2.4
1	A	115	LEU	2.4
1	A	130	TYR	2.4
1	D	325	LEU	2.4
1	D	371	PHE	2.4
2	C	468	PHE	2.4
1	A	101	LEU	2.3
1	D	366	ALA	2.3
2	C	469	GLY	2.3
1	D	274	MET	2.3
1	D	85	VAL	2.3
2	B	493	GLN	2.2
2	B	459	VAL	2.2
2	C	554	ILE	2.2
2	B	607	SER	2.2
2	B	709	ARG	2.2
2	B	487	VAL	2.1
1	D	257	ALA	2.1
1	D	107	ILE	2.1
1	D	196	ILE	2.1
1	D	227	ARG	2.1
2	B	586	GLU	2.1
1	D	341	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	82	VAL	2.1
1	D	151	LEU	2.1
2	C	488	THR	2.1
1	D	379	ILE	2.1
2	C	463	ILE	2.1
1	A	77	GLY	2.1
1	D	141	ILE	2.1
1	D	147	ASP	2.1
2	B	485	LEU	2.0
1	D	94	MET	2.0
1	D	206	LEU	2.0
1	D	374	TRP	2.0
1	D	249	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	D	222	10/11	0.86	0.09	73,81,90,93	0
1	SEP	A	222	10/11	0.89	0.09	73,85,92,113	0

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.

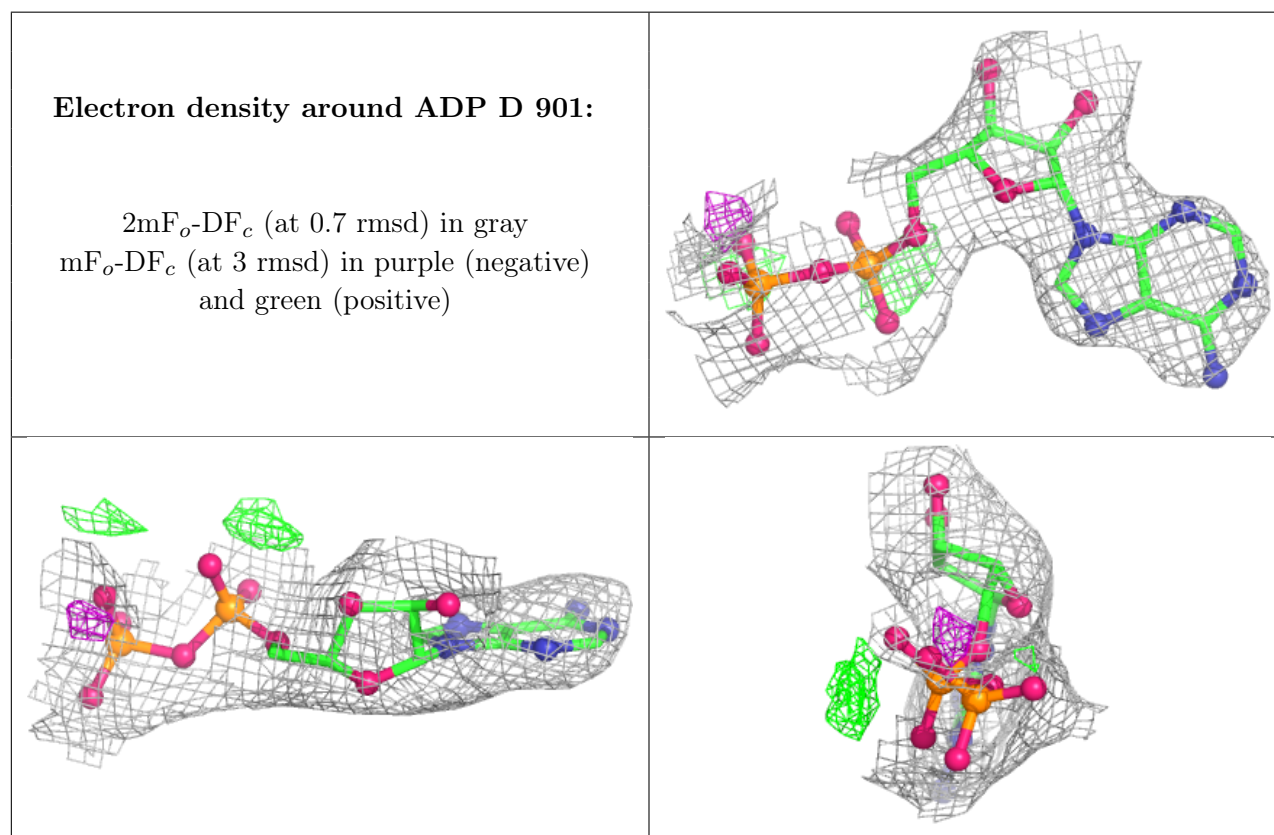
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NA	B	904	1/1	0.64	0.18	92,92,92,92	0
5	GOL	B	905	6/6	0.82	0.15	100,127,145,150	0
4	CA	D	903	1/1	0.88	0.09	108,108,108,108	0

Continued on next page...

Continued from previous page...

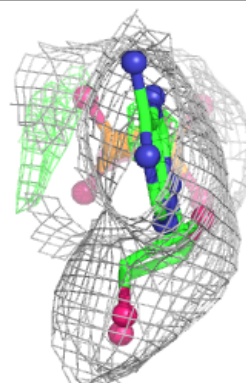
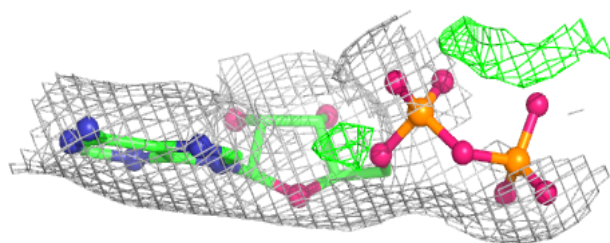
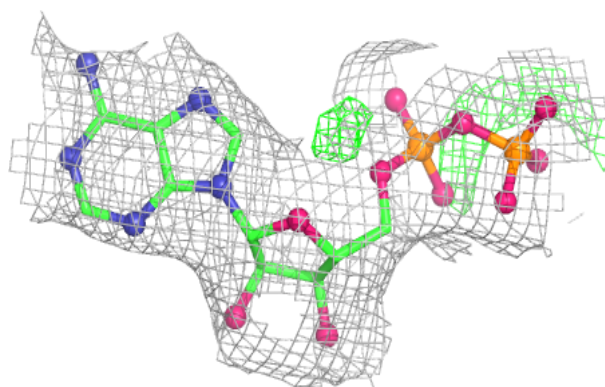
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	D	901	27/27	0.89	0.09	85,96,118,145	0
4	CA	D	902	1/1	0.93	0.08	117,117,117,117	0
3	ADP	A	901	27/27	0.94	0.09	69,82,97,109	0
5	GOL	C	904	6/6	0.95	0.12	43,59,60,67	0
3	ADP	B	901	27/27	0.95	0.08	54,64,77,85	0
4	CA	A	902	1/1	0.95	0.13	95,95,95,95	0
4	CA	B	903	1/1	0.96	0.12	76,76,76,76	0
3	ADP	C	901	27/27	0.96	0.08	47,67,75,96	0
4	CA	A	903	1/1	0.96	0.10	96,96,96,96	0
4	CA	C	903	1/1	0.98	0.10	62,62,62,62	0
4	CA	B	902	1/1	0.98	0.07	63,63,63,63	0
4	CA	C	902	1/1	0.99	0.04	56,56,56,56	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.

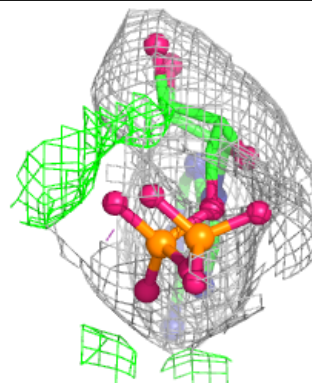
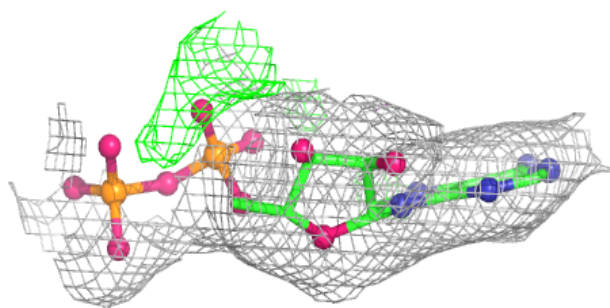
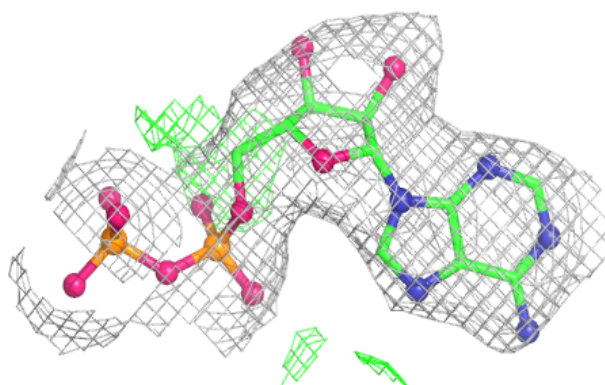


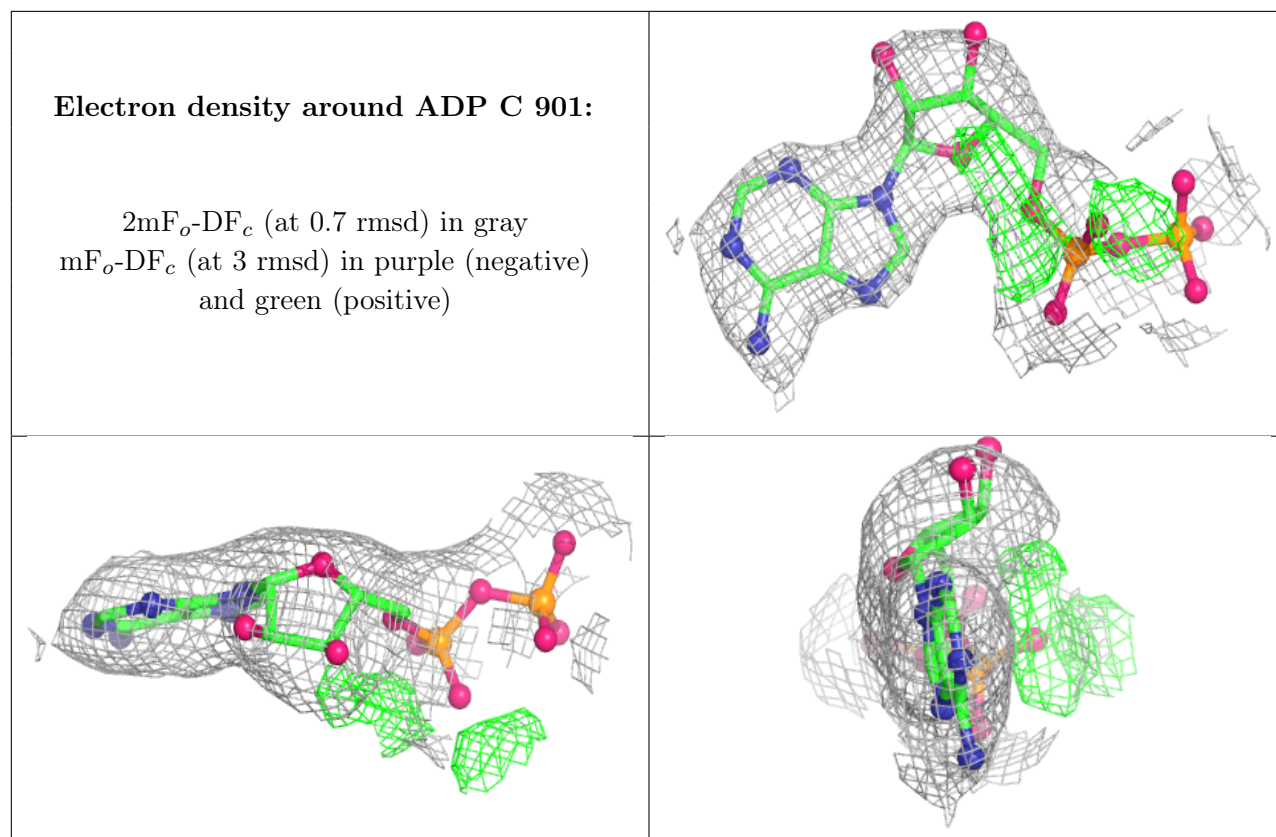
Electron density around ADP A 901:

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

**Electron density around ADP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.