



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:40 PM UTC

PDB ID : 7M7A / pdb_00007m7a
Title : Legionella pneumophila MavQ lipid kinase
Authors : Tomchick, D.R.; Tagliabracci, V.S.; Hsieh, T.S.; Lopez, V.A.
Deposited on : 2021-03-27
Resolution : 3.20 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (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

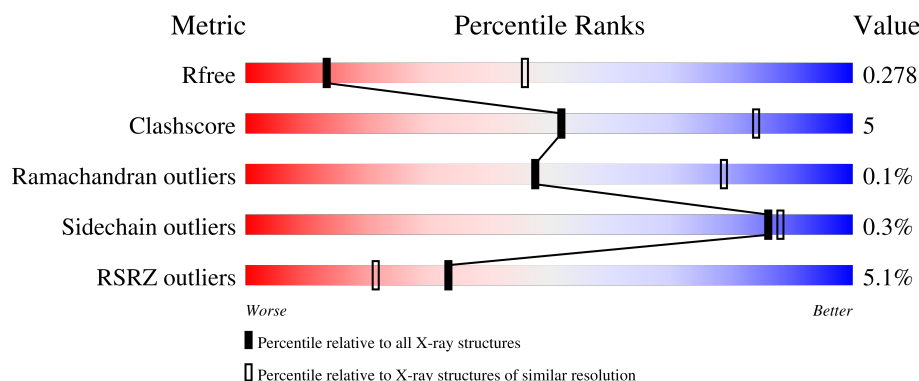
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	590	2% 80% 11% 9%
1	B	590	7% 77% 11% 12%
1	C	590	5% 80% 10% 9%
1	D	590	4% 81% 9% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34843 atoms, of which 17191 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 Phosphoinositide 3-kinase MavQ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	538	Total	C	H	N	O	S	0	0	0
			8775	2852	4336	737	838	12			
1	B	522	Total	C	H	N	O	S	0	0	0
			8516	2770	4211	713	810	12			
1	C	536	Total	C	H	N	O	S	0	0	0
			8754	2844	4328	736	834	12			
1	D	529	Total	C	H	N	O	S	0	0	0
			8638	2809	4268	724	825	12			

There are 40 discrepancies between the modelled and reference sequences:

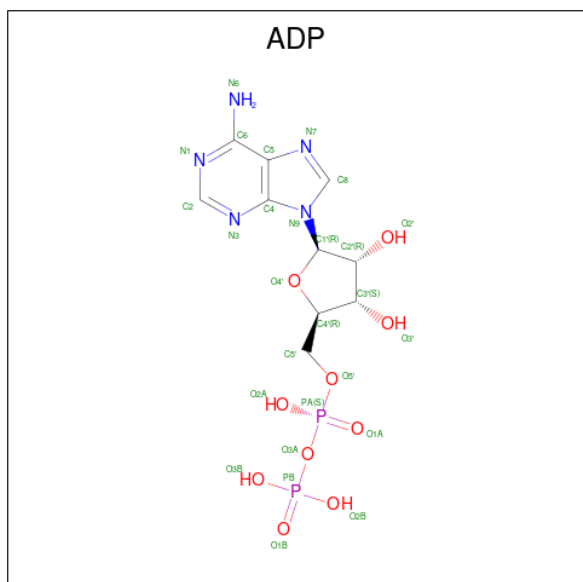
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	SER	-	expression tag	UNP Q5ZRA8
A	-8	GLU	-	expression tag	UNP Q5ZRA8
A	-7	PHE	-	expression tag	UNP Q5ZRA8
A	-6	GLU	-	expression tag	UNP Q5ZRA8
A	-5	LEU	-	expression tag	UNP Q5ZRA8
A	-4	ARG	-	expression tag	UNP Q5ZRA8
A	-3	ARG	-	expression tag	UNP Q5ZRA8
A	-2	GLN	-	expression tag	UNP Q5ZRA8
A	-1	ALA	-	expression tag	UNP Q5ZRA8
A	0	SER	-	expression tag	UNP Q5ZRA8
B	-9	SER	-	expression tag	UNP Q5ZRA8
B	-8	GLU	-	expression tag	UNP Q5ZRA8
B	-7	PHE	-	expression tag	UNP Q5ZRA8
B	-6	GLU	-	expression tag	UNP Q5ZRA8
B	-5	LEU	-	expression tag	UNP Q5ZRA8
B	-4	ARG	-	expression tag	UNP Q5ZRA8
B	-3	ARG	-	expression tag	UNP Q5ZRA8
B	-2	GLN	-	expression tag	UNP Q5ZRA8
B	-1	ALA	-	expression tag	UNP Q5ZRA8
B	0	SER	-	expression tag	UNP Q5ZRA8
C	-9	SER	-	expression tag	UNP Q5ZRA8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP Q5ZRA8
C	-7	PHE	-	expression tag	UNP Q5ZRA8
C	-6	GLU	-	expression tag	UNP Q5ZRA8
C	-5	LEU	-	expression tag	UNP Q5ZRA8
C	-4	ARG	-	expression tag	UNP Q5ZRA8
C	-3	ARG	-	expression tag	UNP Q5ZRA8
C	-2	GLN	-	expression tag	UNP Q5ZRA8
C	-1	ALA	-	expression tag	UNP Q5ZRA8
C	0	SER	-	expression tag	UNP Q5ZRA8
D	-9	SER	-	expression tag	UNP Q5ZRA8
D	-8	GLU	-	expression tag	UNP Q5ZRA8
D	-7	PHE	-	expression tag	UNP Q5ZRA8
D	-6	GLU	-	expression tag	UNP Q5ZRA8
D	-5	LEU	-	expression tag	UNP Q5ZRA8
D	-4	ARG	-	expression tag	UNP Q5ZRA8
D	-3	ARG	-	expression tag	UNP Q5ZRA8
D	-2	GLN	-	expression tag	UNP Q5ZRA8
D	-1	ALA	-	expression tag	UNP Q5ZRA8
D	0	SER	-	expression tag	UNP Q5ZRA8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	
			39	10	12	5	10	2	
2	C	1	Total	C	H	N	O	P	
			39	10	12	5	10	2	
2	D	1	Total	C	H	N	O	P	
			39	10	12	5	10	2	

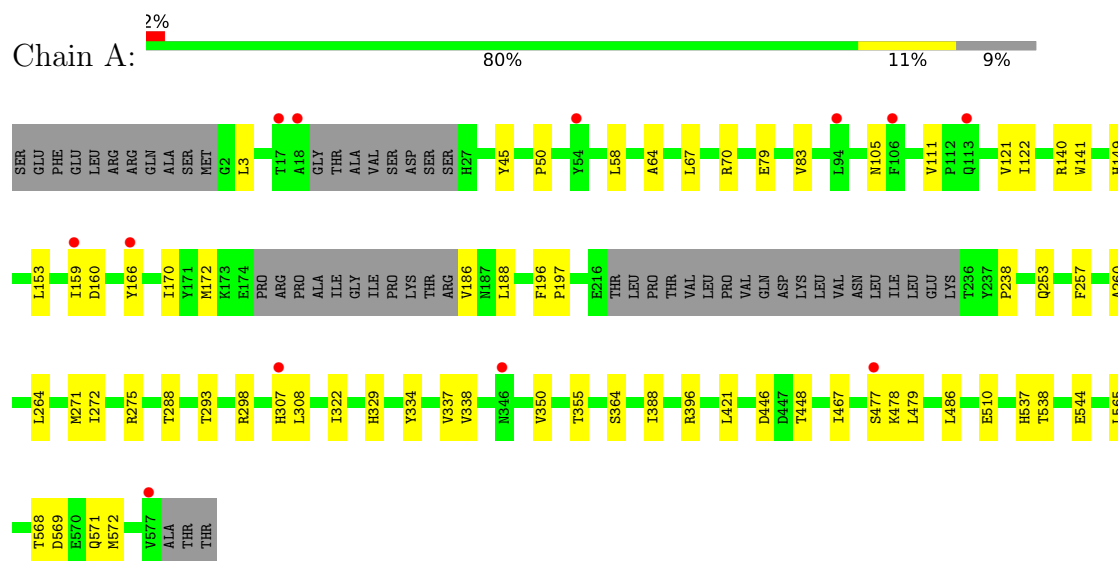
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg		
			1	1	0	0
3	B	1	Total	Mg		
			1	1	0	0
3	C	1	Total	Mg		
			1	1	0	0
3	D	1	Total	Mg		
			1	1	0	0

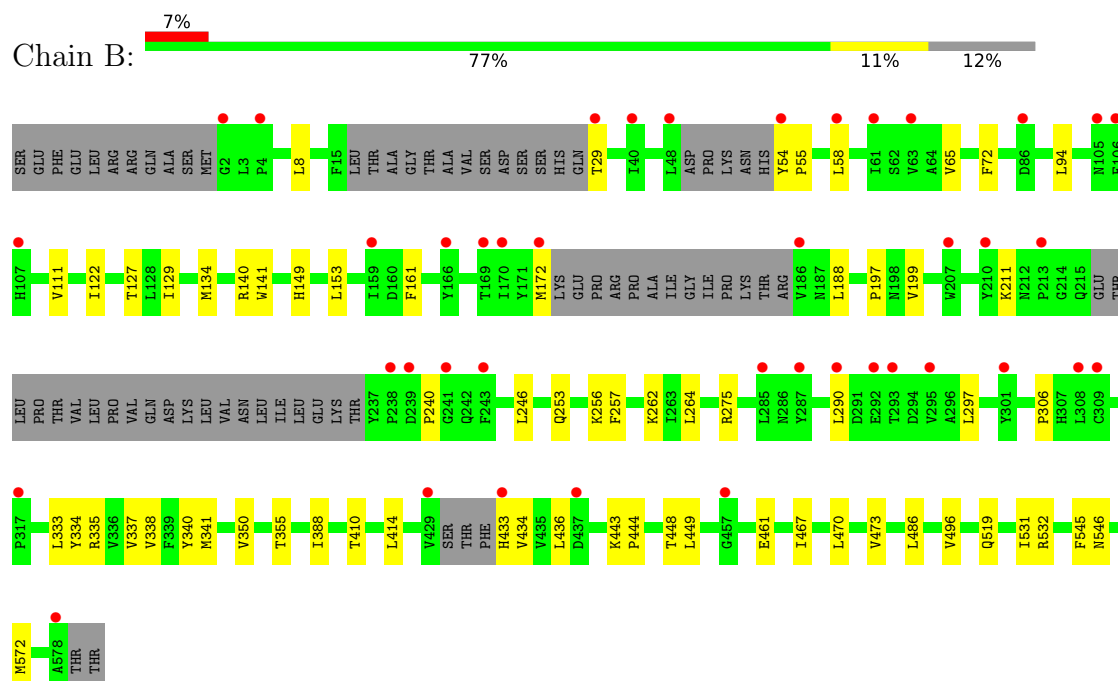
3 Residue-property plots [i](#)

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.

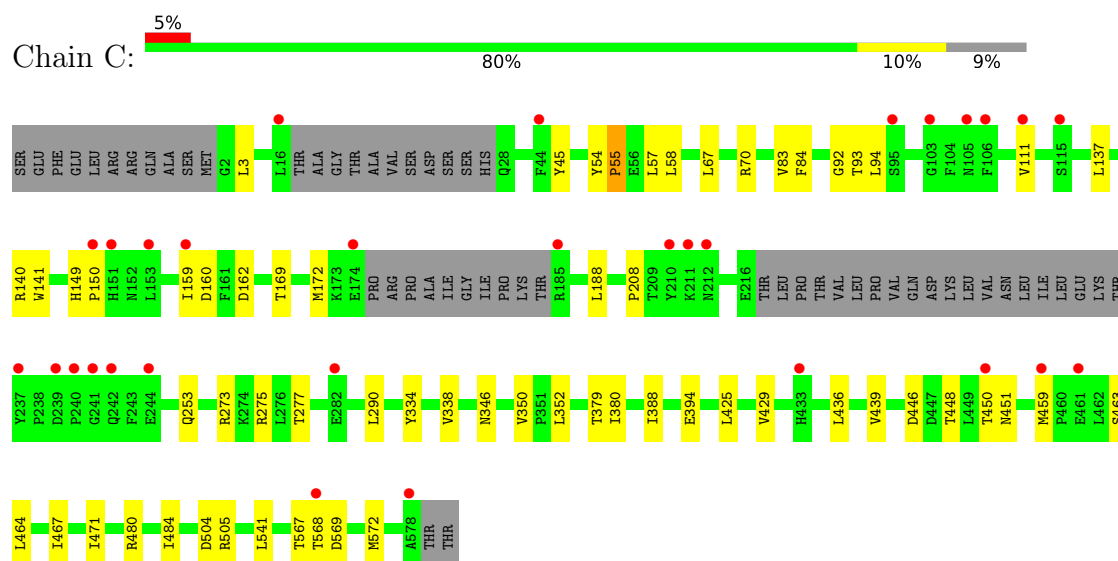
• Molecule 1: Phosphoinositide 3-kinase MavQ



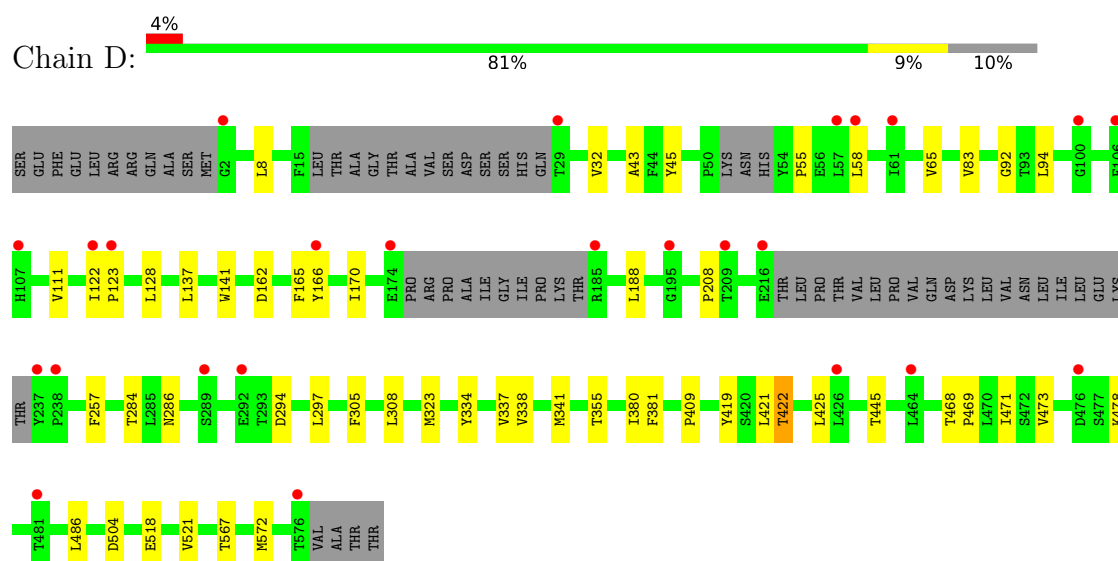
• Molecule 1: Phosphoinositide 3-kinase MavQ



● Molecule 1: Phosphoinositide 3-kinase MavQ



● Molecule 1: Phosphoinositide 3-kinase MavQ



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	69.40Å 210.24Å 499.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 3.20 49.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	80.9 (49.31-3.20) 80.8 (49.31-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.239 , 0.283 0.238 , 0.278	Depositor DCC
R_{free} test set	1995 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	34843	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: ADP, MG

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	0.10	0/4548	0.29	0/6158
1	B	0.10	0/4408	0.29	0/5965
1	C	0.10	0/4534	0.27	0/6137
1	D	0.11	0/4476	0.27	0/6057
All	All	0.10	0/17966	0.28	0/24317

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	4439	4336	4336	46	0
1	B	4305	4211	4211	45	0
1	C	4426	4328	4328	51	0
1	D	4370	4268	4268	38	0
2	A	27	12	12	0	0
2	B	27	12	12	0	0
2	C	27	12	12	0	0
2	D	27	12	12	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	17652	17191	17191	179	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 5.

All (179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ILE:HD11	1:B:545:PHE:CZ	2.16	0.80
1:B:334:TYR:O	1:B:338:VAL:HG12	1.84	0.76
1:D:45:TYR:CE1	1:D:83:VAL:HG21	2.21	0.75
1:A:105:ASN:HB2	1:A:121:VAL:HG12	1.69	0.74
1:D:166:TYR:CE1	1:D:170:ILE:HD13	2.23	0.73
1:C:159:ILE:HD12	1:C:160:ASP:N	2.05	0.71
1:B:434:VAL:HG11	1:B:470:LEU:HD21	1.73	0.69
1:C:45:TYR:CE1	1:C:83:VAL:HG21	2.28	0.69
1:A:166:TYR:CE1	1:A:170:ILE:HD13	2.29	0.68
1:C:429:VAL:CG1	1:C:471:ILE:HG23	2.24	0.68
1:B:253:GLN:HG3	1:B:350:VAL:HG11	1.76	0.68
1:D:137:LEU:HD21	1:D:208:PRO:HG2	1.74	0.68
1:A:159:ILE:HD12	1:A:160:ASP:N	2.09	0.67
1:D:323:MET:HA	1:D:323:MET:HE2	1.79	0.64
1:B:572:MET:HA	1:B:572:MET:HE2	1.79	0.64
1:A:64:ALA:HB3	1:A:322:ILE:HD13	1.80	0.63
1:B:335:ARG:HG2	1:B:449:LEU:HD23	1.80	0.62
1:C:58:LEU:HD12	1:C:172:MET:HB2	1.80	0.62
1:A:166:TYR:HE1	1:A:170:ILE:HD13	1.64	0.62
1:A:257:PHE:HE1	1:A:355:THR:HG22	1.65	0.62
1:D:45:TYR:HE1	1:D:83:VAL:HG21	1.63	0.61
1:A:64:ALA:CB	1:A:322:ILE:HD13	2.30	0.61
1:B:486:LEU:O	1:B:486:LEU:HD23	2.00	0.60
1:A:140:ARG:HD2	1:A:153:LEU:HD21	1.84	0.59
1:A:253:GLN:HG3	1:A:350:VAL:HG11	1.83	0.59
1:A:260:ALA:O	1:A:264:LEU:HD13	2.03	0.59
1:C:67:LEU:HD11	1:C:275:ARG:HG2	1.84	0.59
1:B:134:MET:SD	1:B:256:LYS:HB3	2.43	0.58
1:C:450:THR:HG23	1:C:451:ASN:H	1.68	0.58
1:D:284:THR:HG23	1:D:286:ASN:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:SER:O	1:C:467:ILE:HG22	2.05	0.57
1:A:337:VAL:O	1:A:355:THR:HG21	2.04	0.57
1:A:446:ASP:CG	1:A:448:THR:HG22	2.31	0.56
1:C:429:VAL:HG12	1:C:471:ILE:HG23	1.88	0.56
1:D:468:THR:HA	1:D:471:ILE:HD12	1.89	0.55
1:C:394:GLU:OE2	1:C:505:ARG:NH1	2.40	0.55
1:C:567:THR:OG1	1:C:572:MET:HE2	2.06	0.55
1:A:572:MET:HA	1:A:572:MET:HE2	1.88	0.54
1:C:172:MET:HE2	1:C:290:LEU:HD21	1.89	0.54
1:A:58:LEU:HD12	1:A:172:MET:HB2	1.89	0.53
1:B:140:ARG:HE	1:B:153:LEU:HD21	1.74	0.53
1:C:58:LEU:HD12	1:C:172:MET:CB	2.38	0.53
1:A:45:TYR:CE2	1:A:83:VAL:HG21	2.43	0.53
1:B:264:LEU:HD11	1:B:337:VAL:HG21	1.90	0.53
1:D:83:VAL:HG22	1:D:92:GLY:C	2.34	0.53
1:D:257:PHE:HE1	1:D:355:THR:HG22	1.74	0.53
1:A:122:ILE:HG23	1:A:122:ILE:O	2.09	0.53
1:B:436:LEU:HD11	1:B:467:ILE:HD11	1.91	0.53
1:B:473:VAL:HG12	1:B:473:VAL:O	2.09	0.52
1:B:264:LEU:HD11	1:B:337:VAL:CG2	2.40	0.52
1:D:567:THR:CG2	1:D:572:MET:HE3	2.40	0.52
1:B:436:LEU:HD22	1:B:461:GLU:HB2	1.92	0.52
1:C:58:LEU:HB2	1:C:172:MET:SD	2.50	0.52
1:D:141:TRP:CH2	1:D:188:LEU:HD23	2.45	0.51
1:B:172:MET:CE	1:B:290:LEU:HD21	2.41	0.51
1:B:58:LEU:HB2	1:B:172:MET:SD	2.51	0.51
1:C:45:TYR:HE1	1:C:83:VAL:HG21	1.71	0.51
1:C:137:LEU:HD21	1:C:208:PRO:HG2	1.92	0.51
1:C:425:LEU:CD2	1:C:541:LEU:HD21	2.40	0.51
1:C:464:LEU:HD21	1:C:484:ILE:HG13	1.94	0.50
1:A:477:SER:O	1:A:537:HIS:NE2	2.44	0.50
1:D:257:PHE:CE1	1:D:355:THR:HG22	2.47	0.50
1:D:43:ALA:HB1	1:D:94:LEU:HD22	1.94	0.50
1:A:421:LEU:HD22	1:A:486:LEU:CD2	2.42	0.49
1:C:379:THR:HG22	1:C:380:ILE:HG23	1.94	0.49
1:A:334:TYR:CE1	1:A:338:VAL:HG21	2.47	0.49
1:B:211:LYS:HA	1:B:240:PRO:HG2	1.94	0.49
1:B:531:ILE:HD11	1:B:545:PHE:CE1	2.47	0.49
1:A:67:LEU:HD11	1:A:275:ARG:HG2	1.95	0.49
1:C:439:VAL:HG23	1:C:439:VAL:O	2.12	0.49
1:D:166:TYR:HE1	1:D:170:ILE:HD13	1.74	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ARG:NH2	1:B:388:ILE:O	2.46	0.49
1:C:3:LEU:HD11	1:C:84:PHE:CG	2.47	0.49
1:D:473:VAL:HG12	1:D:473:VAL:O	2.13	0.48
1:D:334:TYR:CE1	1:D:338:VAL:HG21	2.48	0.48
1:C:471:ILE:HG21	1:C:480:ARG:HG3	1.95	0.48
1:D:419:TYR:O	1:D:422:THR:HG22	2.14	0.48
1:D:111:VAL:HG12	1:D:122:ILE:HD11	1.96	0.48
1:C:253:GLN:HG3	1:C:350:VAL:HG11	1.95	0.47
1:B:122:ILE:HG23	1:B:122:ILE:O	2.14	0.47
1:C:141:TRP:CE2	1:C:188:LEU:HD22	2.49	0.47
1:A:479:LEU:HD21	1:A:538:THR:HG21	1.96	0.47
1:C:149:HIS:HB2	1:C:150:PRO:HD2	1.96	0.47
1:B:8:LEU:HD12	1:B:94:LEU:HD12	1.96	0.47
1:B:290:LEU:HD22	1:B:297:LEU:HD23	1.96	0.47
1:D:486:LEU:HD23	1:D:486:LEU:O	2.14	0.47
1:A:275:ARG:NH2	1:A:388:ILE:O	2.47	0.47
1:A:421:LEU:HD12	1:A:544:GLU:HB3	1.96	0.47
1:A:307:HIS:C	1:A:308:LEU:HD12	2.40	0.47
1:C:450:THR:HG23	1:C:451:ASN:N	2.30	0.47
1:C:58:LEU:HD23	1:C:58:LEU:O	2.15	0.47
1:B:29:THR:HG23	1:B:29:THR:O	2.15	0.46
1:B:253:GLN:OE1	1:B:256:LYS:HE3	2.15	0.46
1:A:421:LEU:HD22	1:A:486:LEU:HD22	1.97	0.46
1:C:567:THR:CB	1:C:572:MET:HE2	2.45	0.46
1:B:141:TRP:CE2	1:B:188:LEU:HD22	2.51	0.46
1:B:290:LEU:HD22	1:B:297:LEU:CD2	2.45	0.46
1:B:337:VAL:HG23	1:B:338:VAL:N	2.31	0.46
1:D:421:LEU:HD22	1:D:486:LEU:CD1	2.45	0.46
1:D:421:LEU:HD23	1:D:425:LEU:HD13	1.97	0.46
1:A:271:MET:HG3	1:A:272:ILE:N	2.31	0.46
1:C:504:ASP:OD1	1:C:504:ASP:N	2.49	0.46
1:A:111:VAL:O	1:A:111:VAL:HG23	2.16	0.46
1:C:334:TYR:CE1	1:C:338:VAL:HG21	2.51	0.46
1:C:436:LEU:HD13	1:C:459:MET:CE	2.45	0.46
1:C:58:LEU:HD21	1:C:162:ASP:O	2.15	0.45
1:A:308:LEU:HD12	1:A:308:LEU:N	2.31	0.45
1:A:58:LEU:C	1:A:58:LEU:HD23	2.42	0.45
1:A:141:TRP:CE2	1:A:188:LEU:HD22	2.51	0.45
1:D:123:PRO:HB2	1:D:128:LEU:HD11	1.98	0.45
1:B:433:HIS:O	1:B:433:HIS:ND1	2.49	0.45
1:A:58:LEU:HB2	1:A:172:MET:SD	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ARG:NH1	1:B:546:ASN:OD1	2.50	0.44
1:A:50:PRO:O	1:A:293:THR:HG23	2.16	0.44
1:A:396:ARG:NH1	1:A:565:LEU:HD13	2.32	0.44
1:B:197:PRO:O	1:B:199:VAL:N	2.46	0.44
1:C:275:ARG:NH2	1:C:388:ILE:O	2.50	0.44
1:D:58:LEU:HD21	1:D:162:ASP:O	2.17	0.44
1:B:337:VAL:O	1:B:355:THR:HG21	2.18	0.44
1:B:72:PHE:O	1:B:262:LYS:HE3	2.18	0.43
1:B:111:VAL:O	1:B:111:VAL:HG23	2.19	0.43
1:B:410:THR:O	1:B:414:LEU:HD13	2.18	0.43
1:C:140:ARG:NH2	1:C:160:ASP:O	2.51	0.43
1:D:445:THR:O	1:D:445:THR:HG22	2.18	0.43
1:A:364:SER:HB3	1:A:569:ASP:OD1	2.19	0.43
1:C:425:LEU:HD23	1:C:541:LEU:HD21	2.00	0.43
1:D:8:LEU:HD12	1:D:94:LEU:HD12	1.99	0.43
1:D:504:ASP:N	1:D:504:ASP:OD1	2.46	0.43
1:A:396:ARG:HD3	1:A:510:GLU:OE2	2.18	0.43
1:C:93:THR:HG22	1:C:94:LEU:N	2.34	0.43
1:B:448:THR:O	1:B:448:THR:HG22	2.18	0.43
1:C:169:THR:O	1:C:169:THR:HG22	2.18	0.43
1:A:159:ILE:HD12	1:A:160:ASP:HB2	2.01	0.43
1:D:111:VAL:HG23	1:D:111:VAL:O	2.19	0.43
1:C:111:VAL:HG23	1:C:111:VAL:O	2.18	0.43
1:B:129:ILE:N	1:B:129:ILE:HD12	2.34	0.42
1:C:273:ARG:O	1:C:277:THR:HG23	2.20	0.42
1:D:32:VAL:HG21	1:D:45:TYR:HB2	2.01	0.42
1:A:446:ASP:OD2	1:A:448:THR:HG22	2.19	0.42
1:B:65:VAL:HG21	1:B:161:PHE:HB3	2.01	0.42
1:C:388:ILE:O	1:C:388:ILE:HG12	2.19	0.42
1:A:568:THR:HG22	1:A:569:ASP:N	2.35	0.42
1:C:346:ASN:HB3	1:C:352:LEU:HD13	2.01	0.42
1:A:477:SER:O	1:A:478:LYS:HB2	2.19	0.42
1:C:568:THR:HG22	1:C:569:ASP:N	2.34	0.42
1:C:57:LEU:HD22	1:C:172:MET:HE1	2.00	0.42
1:C:70:ARG:NH2	1:C:380:ILE:HD12	2.35	0.42
1:D:65:VAL:HG12	1:D:165:PHE:HE1	1.84	0.42
1:A:122:ILE:HD12	1:A:238:PRO:HB2	2.01	0.42
1:A:571:GLN:O	1:B:546:ASN:ND2	2.53	0.42
1:B:257:PHE:HE1	1:B:355:THR:HG22	1.84	0.41
1:C:334:TYR:CD1	1:C:338:VAL:HG21	2.55	0.41
1:C:425:LEU:HD21	1:C:541:LEU:HD21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ILE:HG23	1:D:381:PHE:CD1	2.55	0.41
1:B:134:MET:CE	1:B:246:LEU:HB3	2.50	0.41
1:B:340:TYR:O	1:B:341:MET:HE2	2.20	0.41
1:C:436:LEU:HD13	1:C:459:MET:HE2	2.02	0.41
1:A:196:PHE:CG	1:A:197:PRO:HA	2.55	0.41
1:C:83:VAL:HG22	1:C:92:GLY:C	2.46	0.41
1:D:305:PHE:CB	1:D:308:LEU:HD11	2.51	0.41
1:B:54:TYR:N	1:B:55:PRO:HD3	2.35	0.41
1:A:186:VAL:HG21	1:A:329:HIS:CE1	2.55	0.41
1:C:54:TYR:N	1:C:55:PRO:HD3	2.35	0.41
1:D:337:VAL:O	1:D:355:THR:HG21	2.20	0.41
1:D:341:MET:HE3	1:D:409:PRO:HG2	2.03	0.41
1:B:496:VAL:HG21	1:B:519:GLN:HB3	2.02	0.41
1:C:446:ASP:CG	1:C:448:THR:HG22	2.46	0.41
1:D:294:ASP:HB3	1:D:297:LEU:HD13	2.02	0.41
1:A:3:LEU:HD23	1:A:3:LEU:H	1.86	0.41
1:D:43:ALA:CB	1:D:94:LEU:HD22	2.50	0.41
1:D:468:THR:N	1:D:469:PRO:HD2	2.35	0.41
1:D:518:GLU:HA	1:D:521:VAL:HG12	2.02	0.41
1:A:288:THR:HA	1:A:298:ARG:HD3	2.02	0.41
1:B:443:LYS:CG	1:B:444:PRO:HD2	2.50	0.41
1:B:264:LEU:HD21	1:B:333:LEU:HD23	2.04	0.40
1:D:123:PRO:CB	1:D:128:LEU:HD11	2.51	0.40
1:A:70:ARG:CD	1:A:79:GLU:HB3	2.51	0.40
1:C:58:LEU:HD23	1:C:58:LEU:C	2.46	0.40
1:C:94:LEU:HD23	1:C:94:LEU:HA	1.99	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	530/590 (90%)	503 (95%)	27 (5%)	0	100	100
1	B	510/590 (86%)	490 (96%)	19 (4%)	1 (0%)	43	73
1	C	528/590 (90%)	499 (94%)	28 (5%)	1 (0%)	43	73
1	D	519/590 (88%)	492 (95%)	26 (5%)	1 (0%)	43	73
All	All	2087/2360 (88%)	1984 (95%)	100 (5%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	306	PRO
1	D	55	PRO
1	C	55	PRO

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	490/536 (91%)	488 (100%)	2 (0%)	84	86
1	B	474/536 (88%)	472 (100%)	2 (0%)	84	86
1	C	488/536 (91%)	488 (100%)	0	100	100
1	D	482/536 (90%)	480 (100%)	2 (0%)	84	86
All	All	1934/2144 (90%)	1928 (100%)	6 (0%)	86	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	467	ILE
1	B	127	THR
1	B	149	HIS
1	D	422	THR
1	D	478	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	300	GLN
1	A	376	GLN
1	B	151	HIS
1	B	494	HIS
1	C	52	ASN
1	C	151	HIS
1	C	494	HIS
1	D	151	HIS
1	D	312	ASN
1	D	324	ASN
1	D	345	ASN
1	D	376	GLN
1	D	494	HIS
1	D	562	GLN
1	D	564	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	701	3	28,29,29	1.39	4 (14%)	43,45,45	1.88	10 (23%)
2	ADP	C	701	3	28,29,29	1.44	5 (17%)	43,45,45	1.92	11 (25%)
2	ADP	D	701	3	28,29,29	1.39	4 (14%)	43,45,45	1.89	10 (23%)
2	ADP	B	701	3	28,29,29	1.42	5 (17%)	43,45,45	1.85	11 (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
2	ADP	A	701	3	-	3/16/32/32	0/3/3/3
2	ADP	C	701	3	-	10/16/32/32	0/3/3/3
2	ADP	D	701	3	-	7/16/32/32	0/3/3/3
2	ADP	B	701	3	-	5/16/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ADP	C5-C4	4.65	1.47	1.39
2	D	701	ADP	C5-C4	4.63	1.47	1.39
2	B	701	ADP	C5-C4	4.61	1.47	1.39
2	C	701	ADP	C5-C4	4.57	1.47	1.39
2	C	701	ADP	C5-C6	2.73	1.48	1.41
2	B	701	ADP	C5-C6	2.65	1.48	1.41
2	D	701	ADP	C5-C6	2.57	1.48	1.41
2	A	701	ADP	C5-C6	2.52	1.48	1.41
2	C	701	ADP	C8-N7	2.49	1.36	1.31
2	A	701	ADP	C5-N7	-2.46	1.34	1.39
2	C	701	ADP	PA-O3A	2.41	1.62	1.59
2	B	701	ADP	PA-O3A	2.40	1.62	1.59
2	D	701	ADP	C5-N7	-2.36	1.34	1.39
2	B	701	ADP	C8-N7	2.35	1.36	1.31
2	D	701	ADP	C8-N7	2.30	1.36	1.31
2	B	701	ADP	C5-N7	-2.26	1.35	1.39
2	A	701	ADP	C8-N7	2.22	1.35	1.31
2	C	701	ADP	C5-N7	-2.19	1.35	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ADP	C5-C4-N3	-5.91	118.58	126.72
2	D	701	ADP	C5-C4-N3	-5.79	118.74	126.72
2	B	701	ADP	C5-C4-N3	-5.65	118.94	126.72
2	C	701	ADP	C5-C4-N3	-5.61	118.99	126.72
2	A	701	ADP	N3-C4-N9	5.04	135.75	127.17
2	D	701	ADP	N3-C4-N9	4.82	135.37	127.17
2	B	701	ADP	N3-C4-N9	4.61	135.01	127.17
2	C	701	ADP	N3-C4-N9	4.47	134.77	127.17
2	C	701	ADP	C2-N3-C4	3.85	121.24	111.83
2	B	701	ADP	C2-N3-C4	3.81	121.13	111.83
2	D	701	ADP	C2-N3-C4	3.81	121.12	111.83
2	C	701	ADP	N3-C2-N1	-3.77	122.87	128.58
2	A	701	ADP	C2-N3-C4	3.73	120.95	111.83
2	D	701	ADP	N3-C2-N1	-3.71	122.97	128.58
2	B	701	ADP	N3-C2-N1	-3.69	123.00	128.58
2	C	701	ADP	C4-C5-N7	-3.54	106.54	110.58
2	A	701	ADP	N3-C2-N1	-3.52	123.26	128.58
2	B	701	ADP	C4-C5-N7	-3.30	106.81	110.58
2	D	701	ADP	C4-C5-N7	-3.17	106.95	110.58
2	C	701	ADP	C4-N9-C8	3.12	109.01	105.74
2	B	701	ADP	C4-N9-C8	3.01	108.90	105.74
2	A	701	ADP	C4-N9-C8	2.99	108.87	105.74
2	A	701	ADP	C4-C5-N7	-2.98	107.17	110.58
2	D	701	ADP	C4-N9-C8	2.96	108.85	105.74
2	C	701	ADP	C5-N7-C8	2.75	107.77	103.45
2	B	701	ADP	C5-N7-C8	2.62	107.56	103.45
2	D	701	ADP	C5-N7-C8	2.60	107.53	103.45
2	D	701	ADP	C3'-C2'-C1'	2.58	106.35	101.46
2	A	701	ADP	C5-N7-C8	2.52	107.41	103.45
2	A	701	ADP	C3'-C2'-C1'	2.51	106.22	101.46
2	C	701	ADP	N9-C8-N7	-2.46	110.44	113.94
2	B	701	ADP	C3'-C2'-C1'	2.45	106.11	101.46
2	C	701	ADP	C6-C5-N7	2.31	136.54	132.09
2	B	701	ADP	N9-C8-N7	-2.29	110.68	113.94
2	C	701	ADP	C3'-C2'-C1'	2.23	105.69	101.46
2	D	701	ADP	N9-C8-N7	-2.23	110.78	113.94
2	A	701	ADP	N9-C8-N7	-2.16	110.87	113.94
2	D	701	ADP	C2-N1-C6	2.15	122.27	118.73
2	B	701	ADP	C6-C5-N7	2.14	136.21	132.09
2	C	701	ADP	C2-N1-C6	2.06	122.11	118.73
2	B	701	ADP	C2-N1-C6	2.04	122.08	118.73
2	A	701	ADP	C2-N1-C6	2.03	122.06	118.73

There are no chirality outliers.

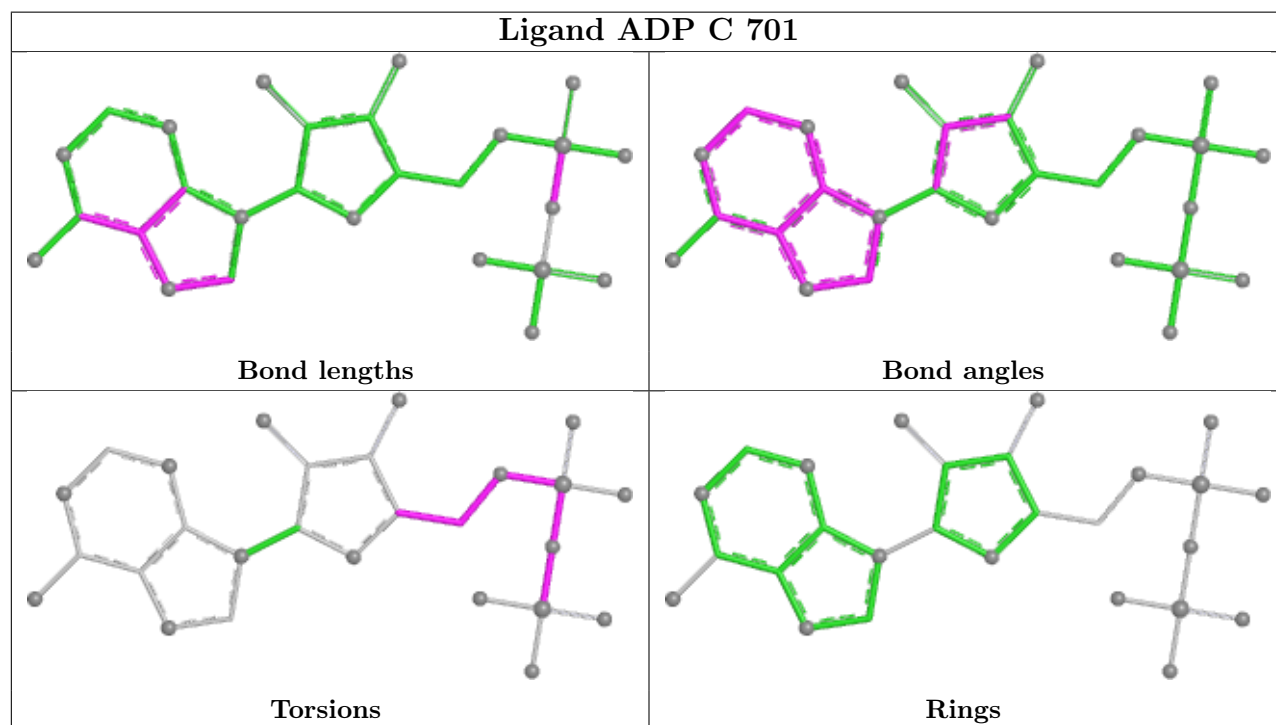
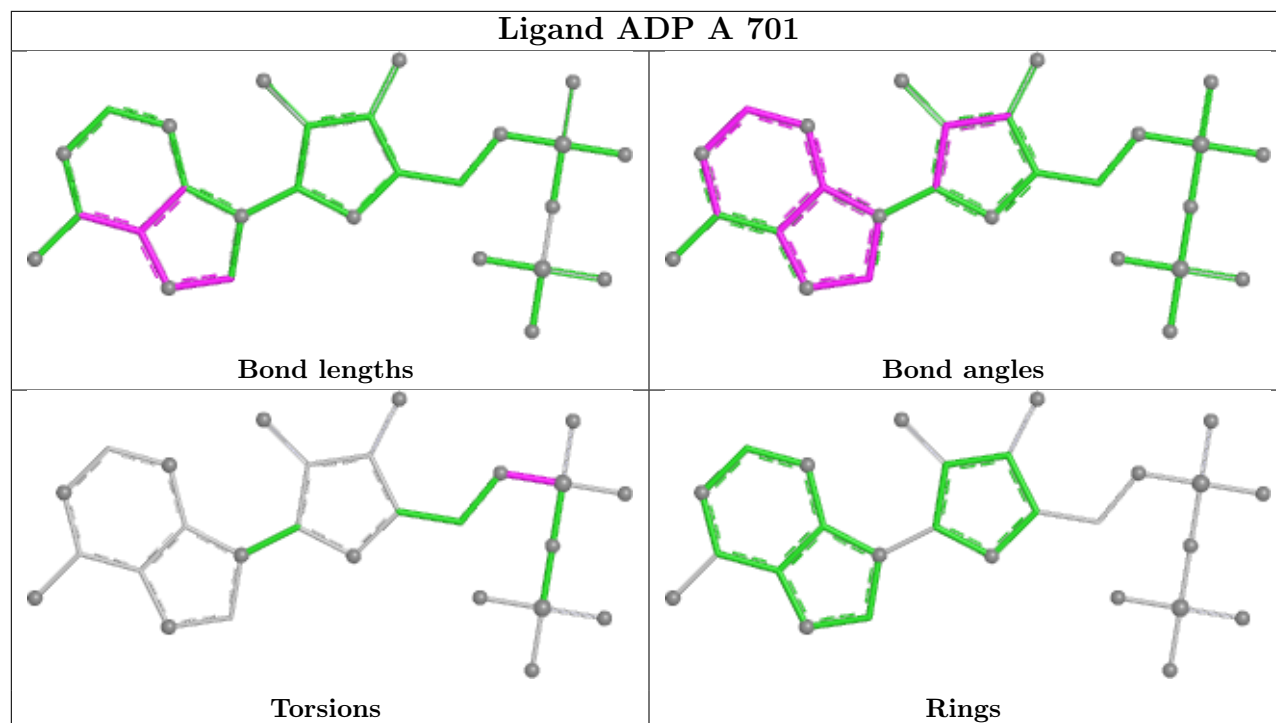
All (25) torsion outliers are listed below:

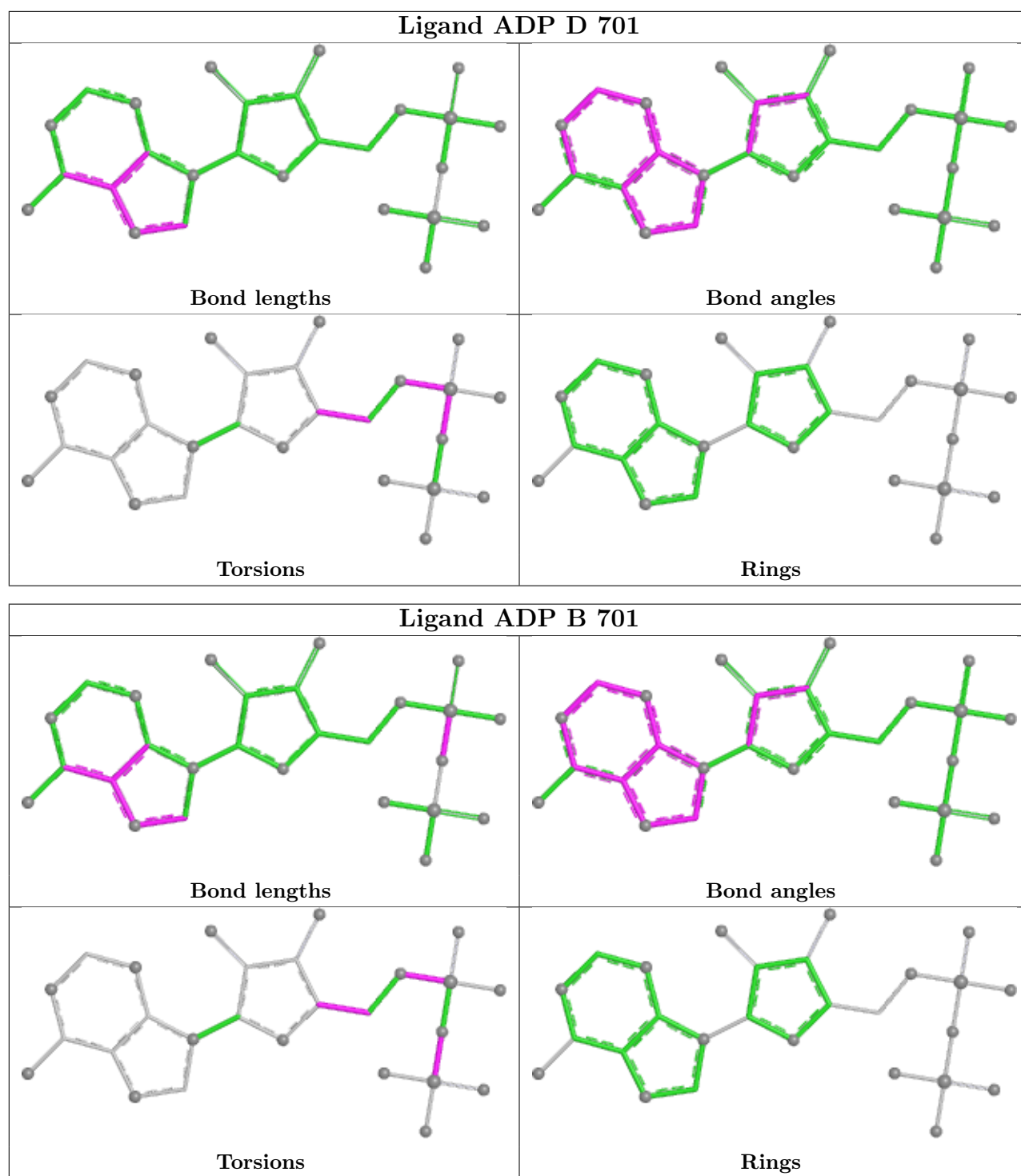
Mol	Chain	Res	Type	Atoms
2	B	701	ADP	PA-O3A-PB-O2B
2	B	701	ADP	C5'-O5'-PA-O1A
2	B	701	ADP	O4'-C4'-C5'-O5'
2	B	701	ADP	C3'-C4'-C5'-O5'
2	C	701	ADP	PA-O3A-PB-O2B
2	C	701	ADP	C5'-O5'-PA-O1A
2	C	701	ADP	C5'-O5'-PA-O2A
2	C	701	ADP	C3'-C4'-C5'-O5'
2	D	701	ADP	O4'-C4'-C5'-O5'
2	D	701	ADP	C3'-C4'-C5'-O5'
2	C	701	ADP	O4'-C4'-C5'-O5'
2	C	701	ADP	PB-O3A-PA-O2A
2	C	701	ADP	C4'-C5'-O5'-PA
2	A	701	ADP	C5'-O5'-PA-O1A
2	A	701	ADP	C5'-O5'-PA-O2A
2	A	701	ADP	C5'-O5'-PA-O3A
2	B	701	ADP	C5'-O5'-PA-O3A
2	C	701	ADP	C5'-O5'-PA-O3A
2	D	701	ADP	C5'-O5'-PA-O1A
2	D	701	ADP	C5'-O5'-PA-O2A
2	D	701	ADP	C5'-O5'-PA-O3A
2	C	701	ADP	PA-O3A-PB-O1B
2	D	701	ADP	PB-O3A-PA-O1A
2	D	701	ADP	PB-O3A-PA-O2A
2	C	701	ADP	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	538/590 (91%)	0.16	12 (2%) 62 42	18, 50, 94, 122	0
1	B	522/590 (88%)	0.61	41 (7%) 18 12	23, 69, 121, 151	0
1	C	536/590 (90%)	0.42	30 (5%) 30 19	23, 59, 97, 122	0
1	D	529/590 (89%)	0.54	25 (4%) 36 23	33, 71, 114, 141	0
All	All	2125/2360 (90%)	0.43	108 (5%) 33 21	18, 62, 108, 151	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	PHE	5.2
1	D	2	GLY	4.5
1	C	212	ASN	4.4
1	A	166	TYR	4.4
1	D	209	THR	4.1
1	B	309	CYS	4.0
1	B	29	THR	3.9
1	B	238	PRO	3.8
1	A	18	ALA	3.8
1	B	58	LEU	3.8
1	D	289	SER	3.6
1	C	106	PHE	3.6
1	B	166	TYR	3.6
1	B	2	GLY	3.5
1	D	166	TYR	3.4
1	B	159	ILE	3.4
1	B	578	ALA	3.3
1	D	464	LEU	3.3
1	C	241	GLY	3.3
1	B	186	VAL	3.2
1	A	577	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	151	HIS	3.0
1	B	290	LEU	2.9
1	D	58	LEU	2.9
1	C	103	GLY	2.9
1	B	107	HIS	2.9
1	B	308	LEU	2.9
1	C	105	ASN	2.9
1	D	123	PRO	2.8
1	B	239	ASP	2.8
1	B	437	ASP	2.8
1	A	113	GLN	2.8
1	C	239	ASP	2.8
1	B	243	PHE	2.8
1	C	237	TYR	2.8
1	A	477	SER	2.8
1	B	292	GLU	2.8
1	C	433	HIS	2.7
1	C	461	GLU	2.7
1	A	346	ASN	2.7
1	D	292	GLU	2.6
1	A	307	HIS	2.6
1	A	159	ILE	2.6
1	B	293	THR	2.6
1	D	576	THR	2.6
1	C	450	THR	2.6
1	D	107	HIS	2.6
1	B	457	GLY	2.6
1	C	568	THR	2.6
1	B	105	ASN	2.5
1	C	240	PRO	2.5
1	D	476	ASP	2.5
1	B	433	HIS	2.5
1	B	4	PRO	2.5
1	D	237	TYR	2.5
1	D	426	LEU	2.5
1	D	195	GLY	2.5
1	B	106	PHE	2.4
1	C	211	LYS	2.4
1	C	159	ILE	2.4
1	B	172	MET	2.4
1	D	61	ILE	2.4
1	B	207	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	115	SER	2.4
1	C	578	ALA	2.3
1	B	429	VAL	2.3
1	B	170	ILE	2.3
1	C	185	ARG	2.3
1	D	185	ARG	2.3
1	D	57	LEU	2.3
1	D	216	GLU	2.3
1	B	63	VAL	2.3
1	B	295	VAL	2.3
1	C	282	GLU	2.3
1	D	238	PRO	2.3
1	D	174	GLU	2.2
1	B	61	ILE	2.2
1	C	111	VAL	2.2
1	C	242	GLN	2.2
1	B	48	LEU	2.2
1	C	459	MET	2.2
1	B	169	THR	2.2
1	B	301	TYR	2.2
1	D	122	ILE	2.2
1	C	153	LEU	2.2
1	B	86	ASP	2.2
1	C	16	LEU	2.1
1	A	54	TYR	2.1
1	B	54	TYR	2.1
1	C	174	GLU	2.1
1	C	44	PHE	2.1
1	A	94	LEU	2.1
1	D	481	THR	2.1
1	D	100	GLY	2.1
1	D	29	THR	2.1
1	B	241	GLY	2.1
1	A	106	PHE	2.1
1	B	317	PRO	2.1
1	C	95	SER	2.1
1	B	287	TYR	2.1
1	B	210	TYR	2.0
1	C	210	TYR	2.0
1	B	40	ILE	2.0
1	A	17	THR	2.0
1	B	213	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	150	PRO	2.0
1	C	244	GLU	2.0
1	B	285	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

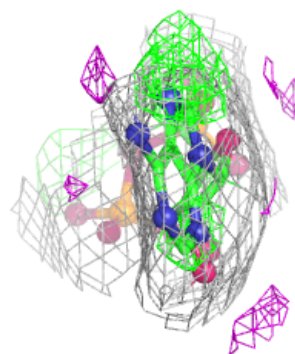
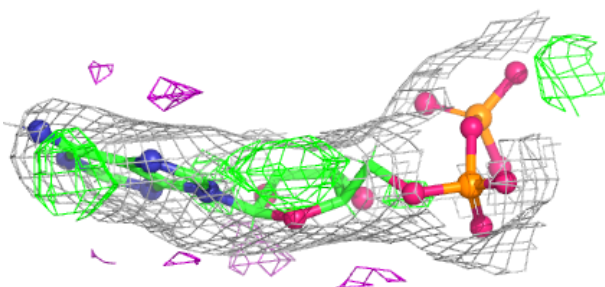
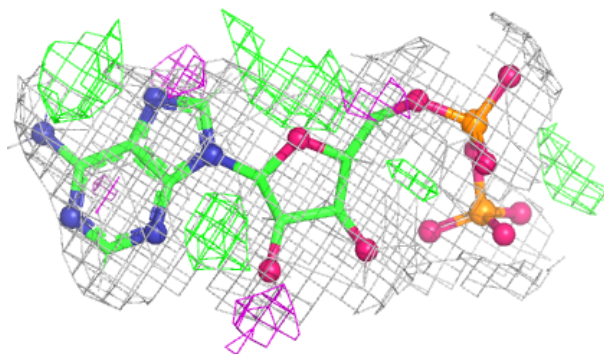
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	C	701	27/27	0.80	0.16	48,72,97,100	0
2	ADP	A	701	27/27	0.83	0.14	48,64,90,101	0
2	ADP	D	701	27/27	0.85	0.12	47,66,105,109	0
3	MG	C	702	1/1	0.85	0.24	58,58,58,58	0
2	ADP	B	701	27/27	0.87	0.11	49,70,97,108	0
3	MG	A	702	1/1	0.90	0.17	57,57,57,57	0
3	MG	B	702	1/1	0.91	0.18	62,62,62,62	0
3	MG	D	702	1/1	0.93	0.15	72,72,72,72	0

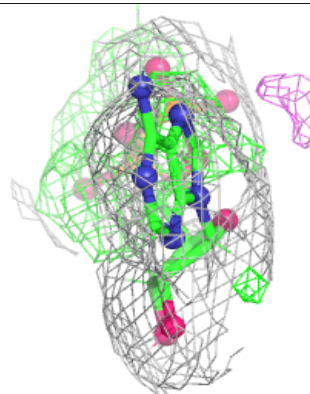
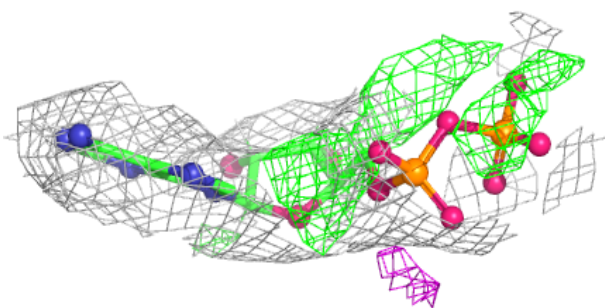
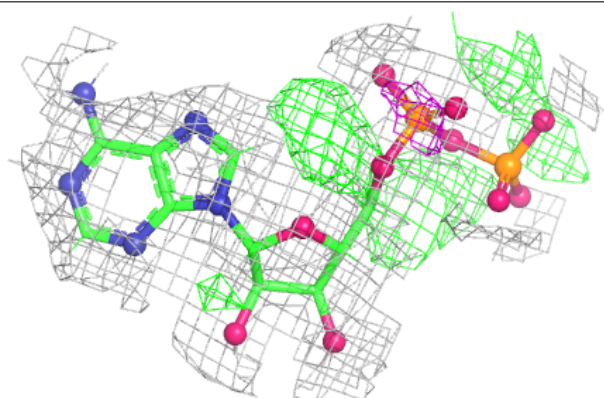
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 701:

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

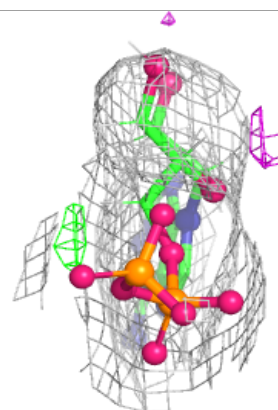
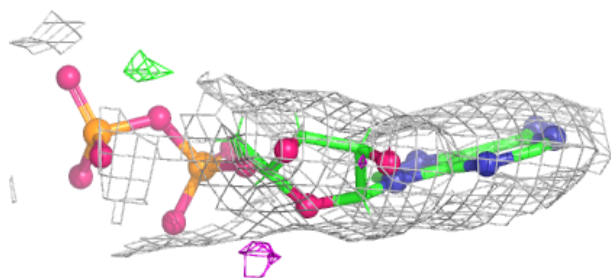
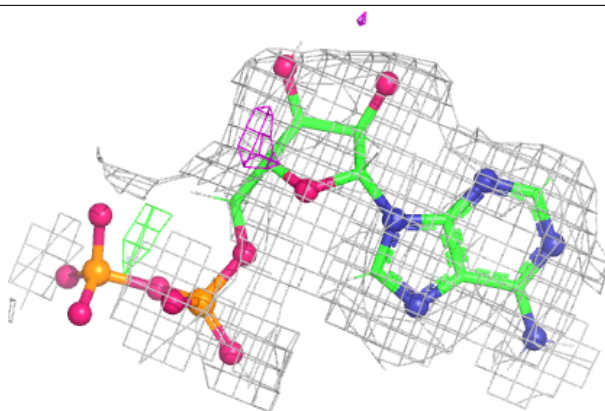
**Electron density around ADP A 701:**

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



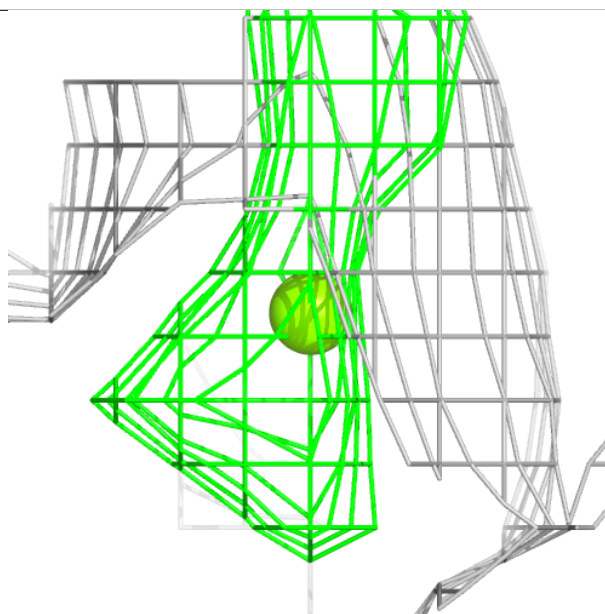
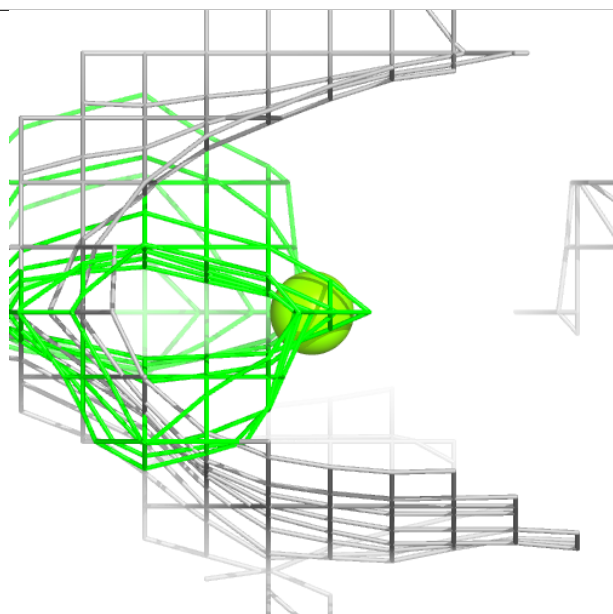
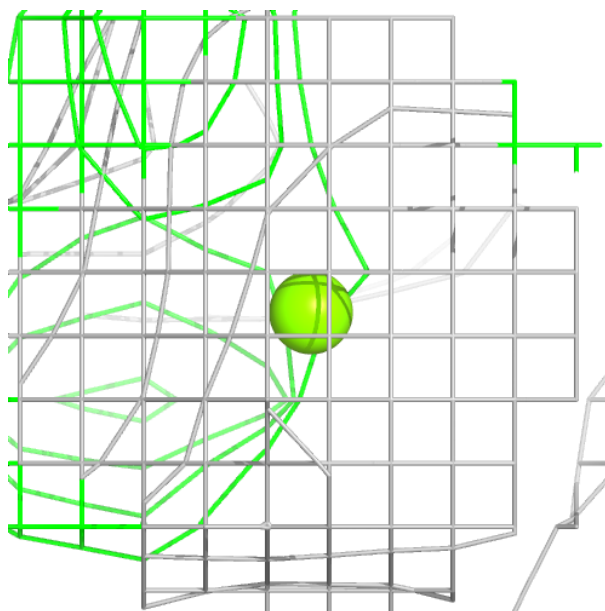
Electron density around ADP D 701:

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



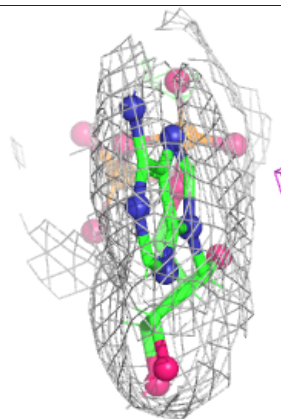
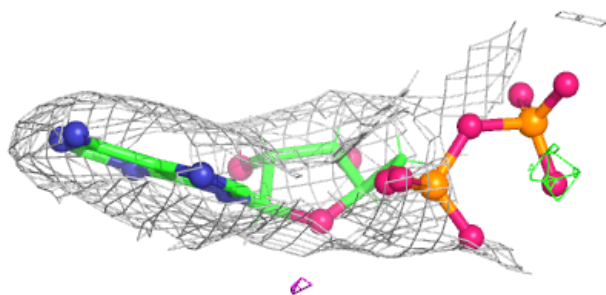
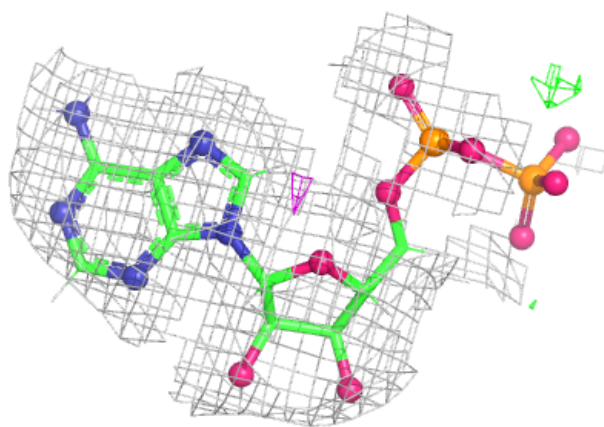
Electron density around MG C 702:

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



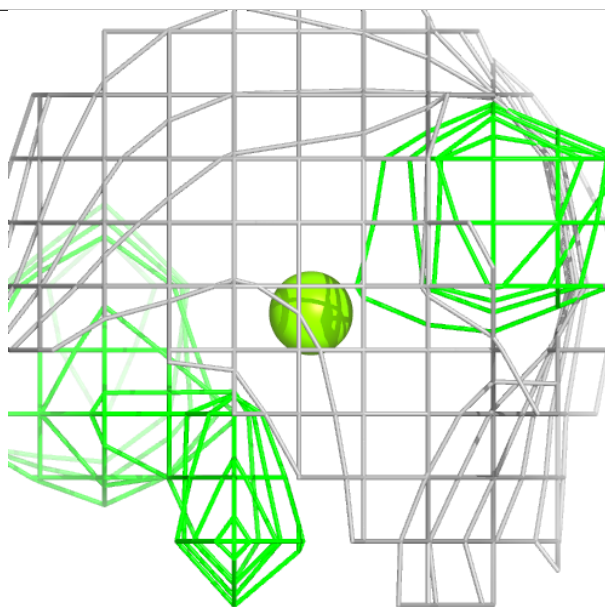
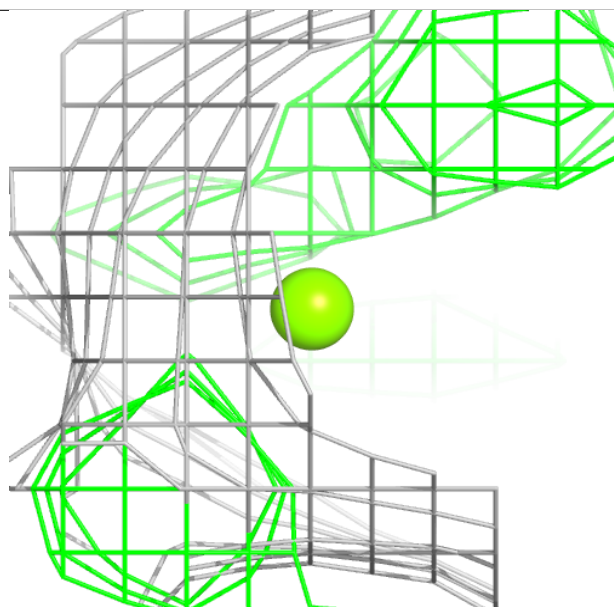
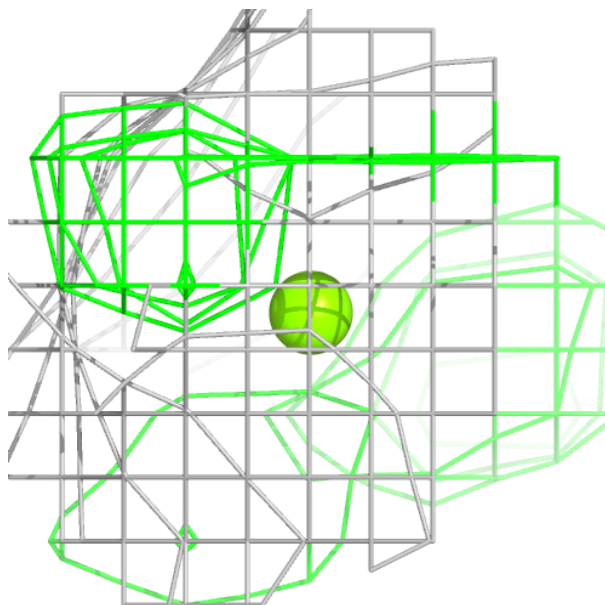
Electron density around ADP B 701:

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



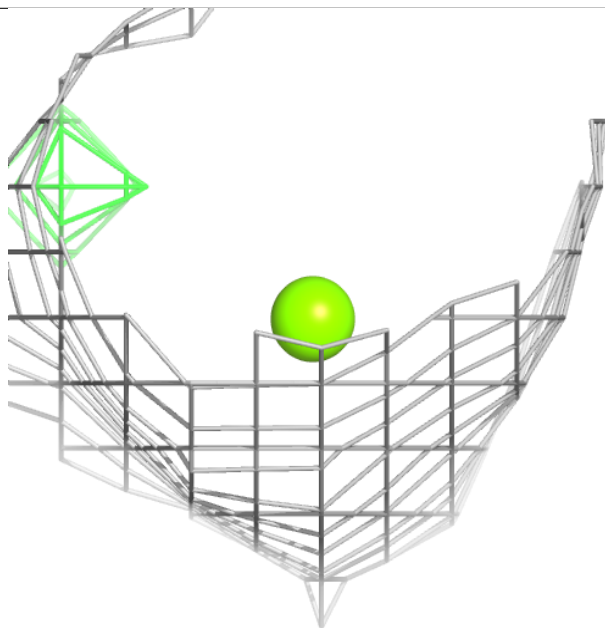
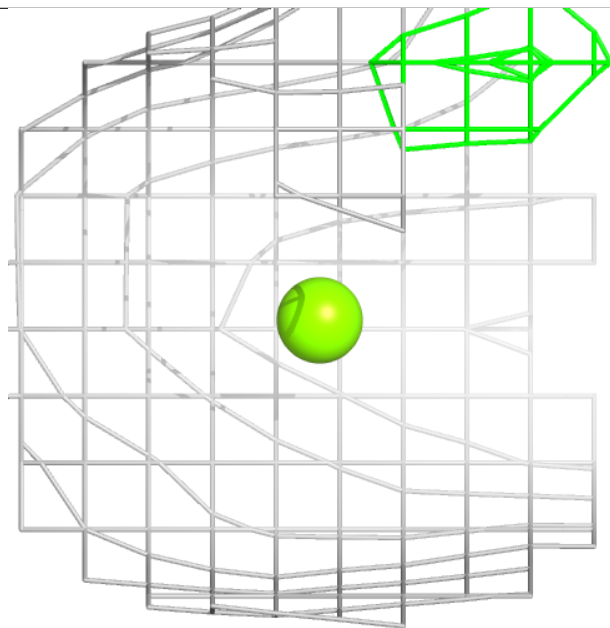
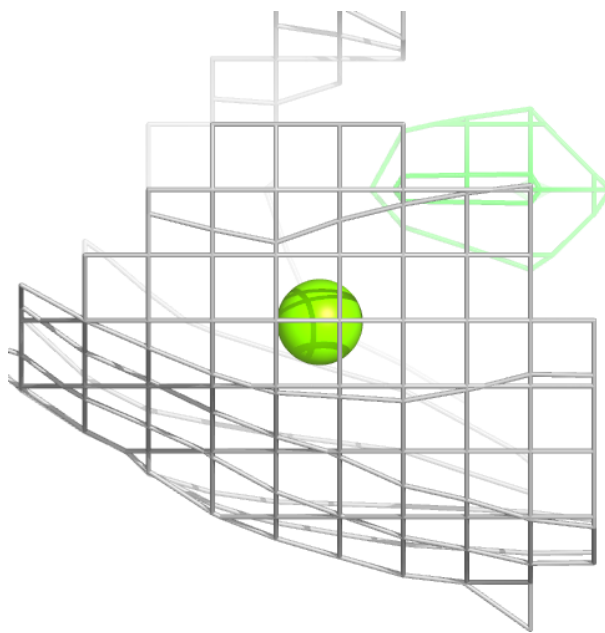
Electron density around MG A 702:

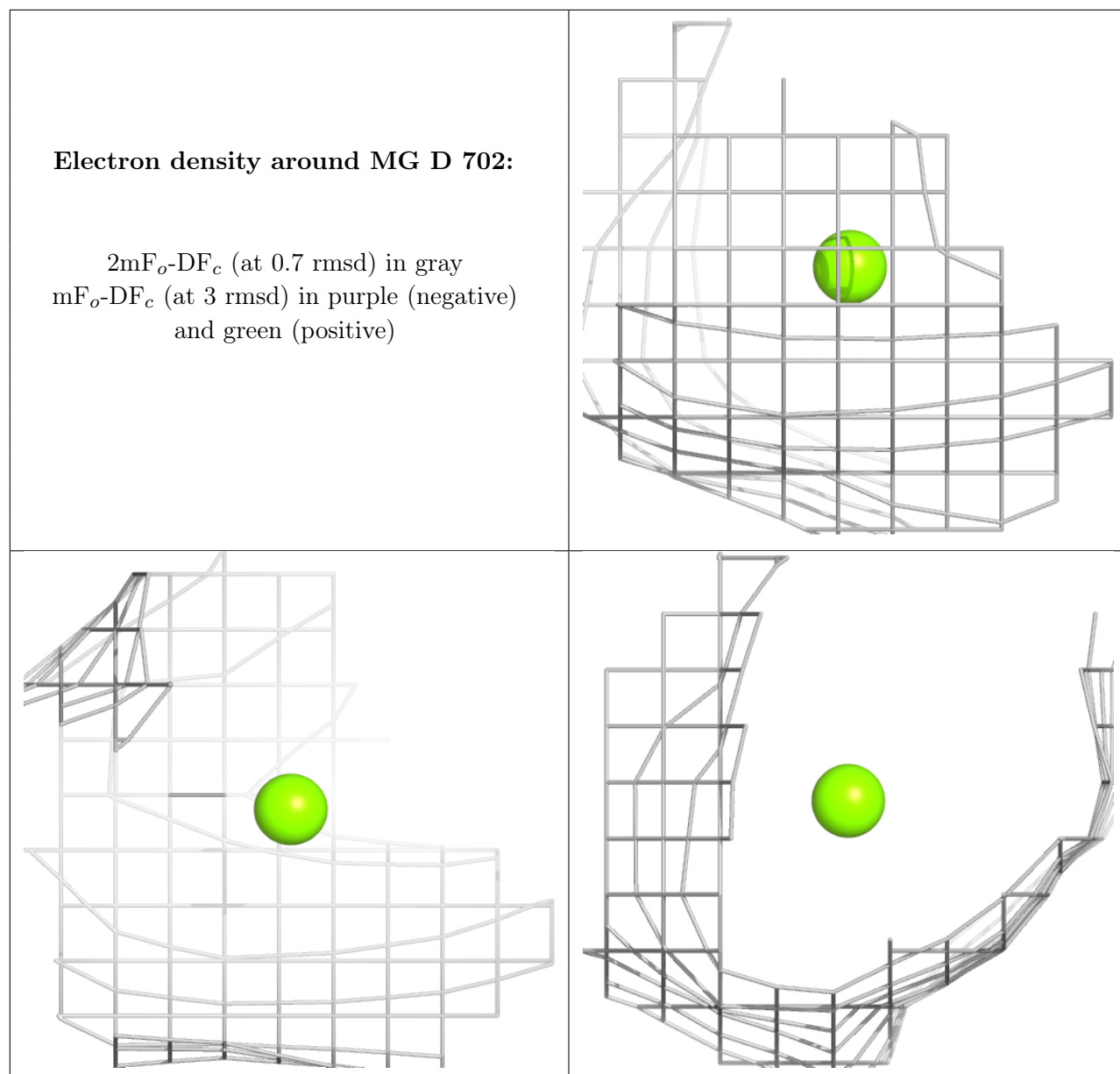
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 702:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.