



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 AM UTC

PDB ID : 6PAR / pdb_00006par
Title : Structure of a bacterial Atm1-family ABC exporter with MgAMPPNP bound
Authors : Fan, C.; Kaiser, J.T.; Rees, D.C.
Deposited on : 2019-06-11
Resolution : 3.35 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

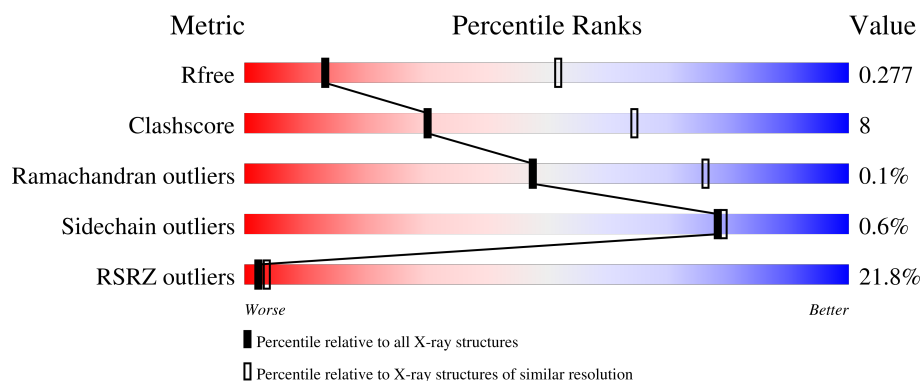
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	614	8% 80% 14% 6%
1	B	614	9% 76% 19% 5%
1	C	614	23% 72% 20% 7%
1	D	614	28% 75% 18% 7%
1	E	614	26% 72% 20% 8%

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Mol	Chain	Length	Quality of chain
1	F	614	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26975 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 ATM1-type heavy metal exporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4489	2868	796	813	12			
1	B	584	Total	C	N	O	S	0	0	0
			4542	2903	805	822	12			
1	C	573	Total	C	N	O	S	0	0	0
			4443	2837	788	806	12			
1	D	573	Total	C	N	O	S	0	0	0
			4438	2830	788	808	12			
1	E	565	Total	C	N	O	S	0	0	0
			4376	2792	778	794	12			
1	F	579	Total	C	N	O	S	0	0	0
			4495	2871	797	815	12			

There are 36 discrepancies between the modelled and reference sequences:

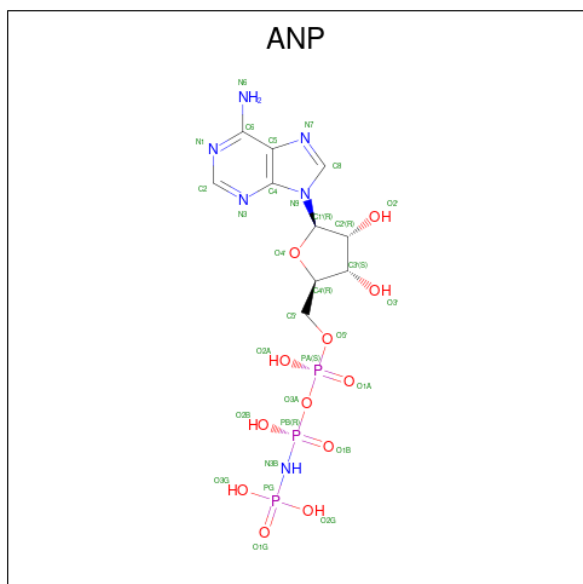
Chain	Residue	Modelled	Actual	Comment	Reference
A	609	HIS	-	expression tag	UNP Q2G506
A	610	HIS	-	expression tag	UNP Q2G506
A	611	HIS	-	expression tag	UNP Q2G506
A	612	HIS	-	expression tag	UNP Q2G506
A	613	HIS	-	expression tag	UNP Q2G506
A	614	HIS	-	expression tag	UNP Q2G506
B	609	HIS	-	expression tag	UNP Q2G506
B	610	HIS	-	expression tag	UNP Q2G506
B	611	HIS	-	expression tag	UNP Q2G506
B	612	HIS	-	expression tag	UNP Q2G506
B	613	HIS	-	expression tag	UNP Q2G506
B	614	HIS	-	expression tag	UNP Q2G506
C	609	HIS	-	expression tag	UNP Q2G506
C	610	HIS	-	expression tag	UNP Q2G506
C	611	HIS	-	expression tag	UNP Q2G506
C	612	HIS	-	expression tag	UNP Q2G506
C	613	HIS	-	expression tag	UNP Q2G506

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Chain	Residue	Modelled	Actual	Comment	Reference
C	614	HIS	-	expression tag	UNP Q2G506
D	609	HIS	-	expression tag	UNP Q2G506
D	610	HIS	-	expression tag	UNP Q2G506
D	611	HIS	-	expression tag	UNP Q2G506
D	612	HIS	-	expression tag	UNP Q2G506
D	613	HIS	-	expression tag	UNP Q2G506
D	614	HIS	-	expression tag	UNP Q2G506
E	609	HIS	-	expression tag	UNP Q2G506
E	610	HIS	-	expression tag	UNP Q2G506
E	611	HIS	-	expression tag	UNP Q2G506
E	612	HIS	-	expression tag	UNP Q2G506
E	613	HIS	-	expression tag	UNP Q2G506
E	614	HIS	-	expression tag	UNP Q2G506
F	609	HIS	-	expression tag	UNP Q2G506
F	610	HIS	-	expression tag	UNP Q2G506
F	611	HIS	-	expression tag	UNP Q2G506
F	612	HIS	-	expression tag	UNP Q2G506
F	613	HIS	-	expression tag	UNP Q2G506
F	614	HIS	-	expression tag	UNP Q2G506

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

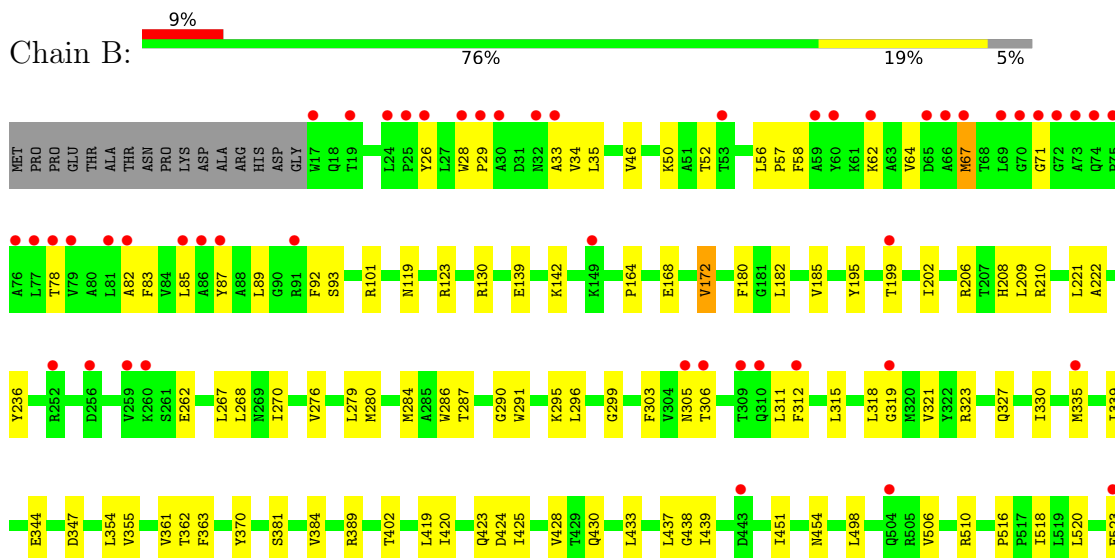
3 Residue-property plots [i](#)

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: ATM1-type heavy metal exporter

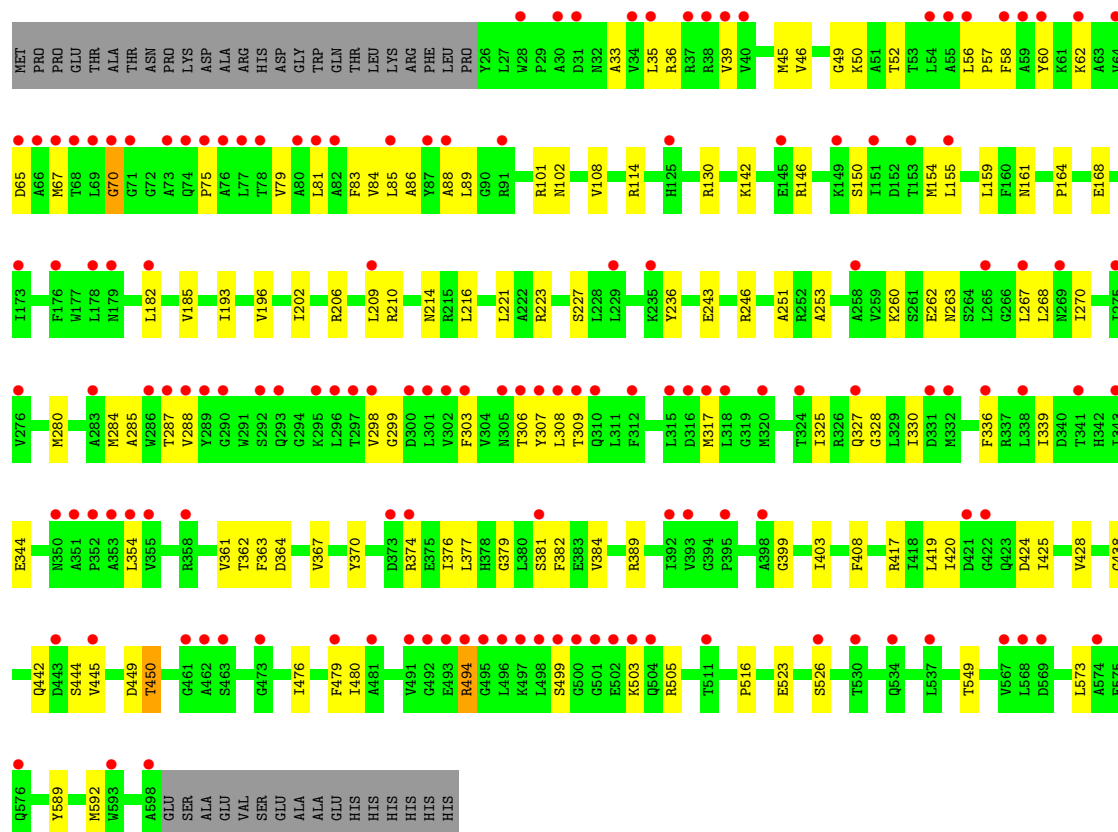
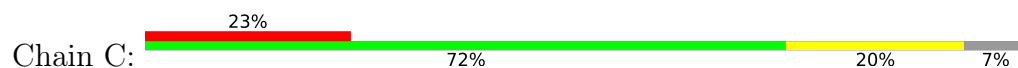


• Molecule 1: ATM1-type heavy metal exporter

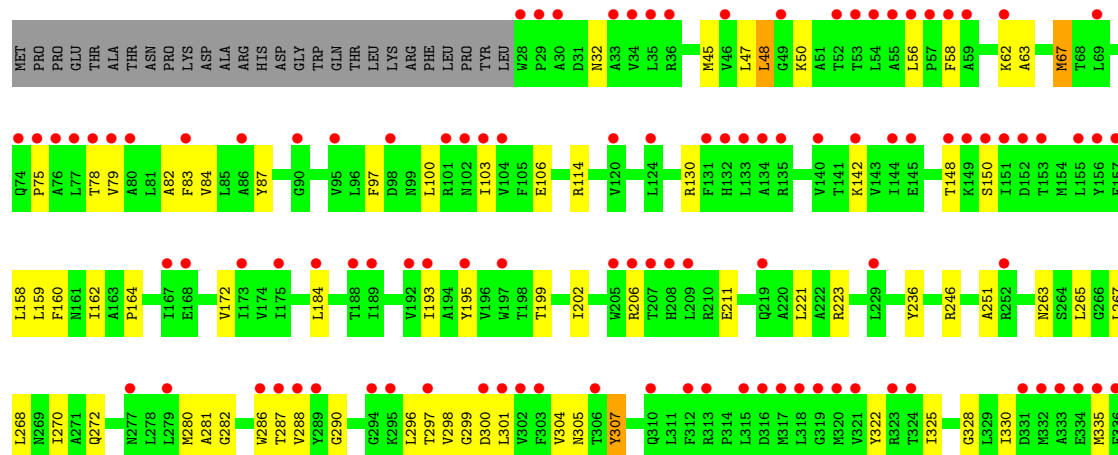
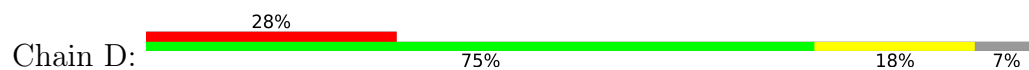


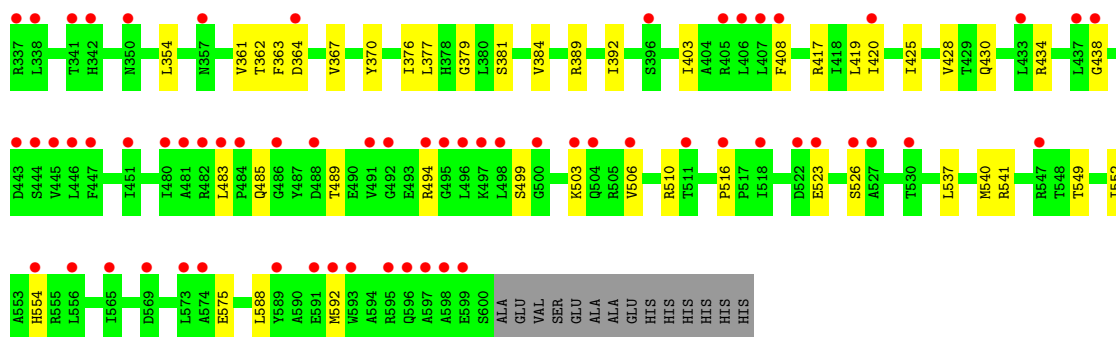


• Molecule 1: ATM1-type heavy metal exporter

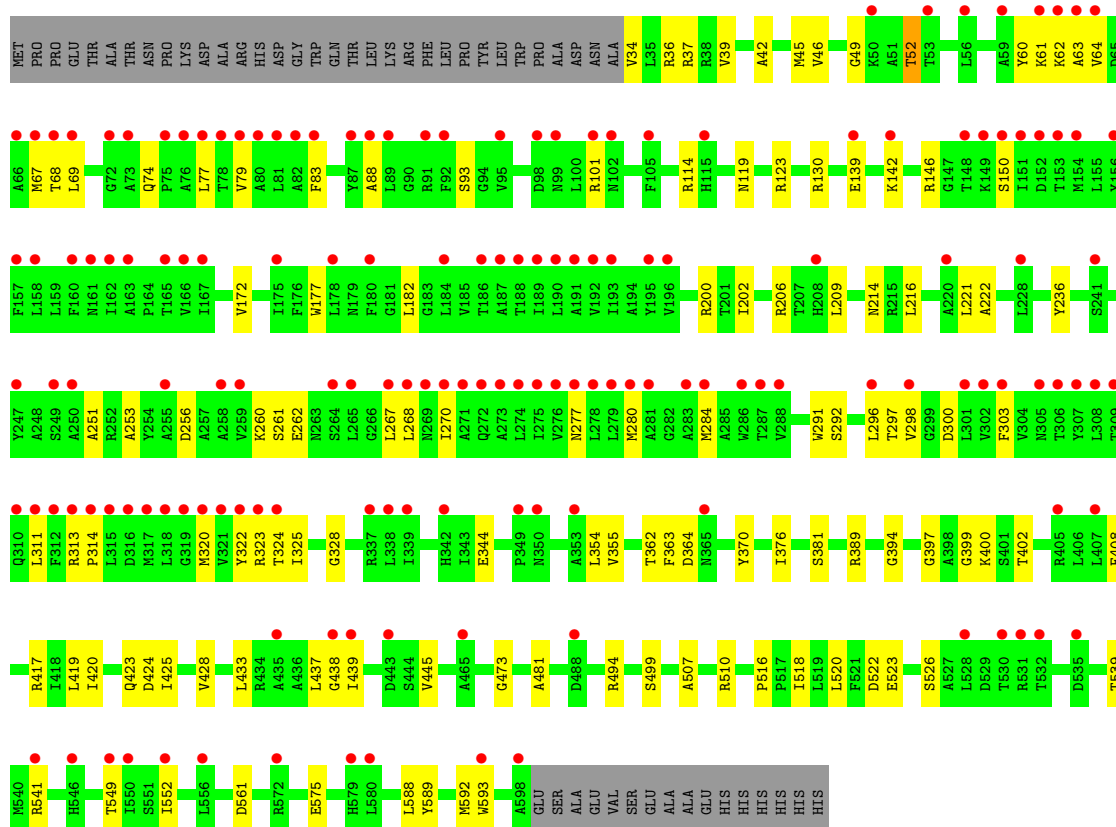


• Molecule 1: ATM1-type heavy metal exporter

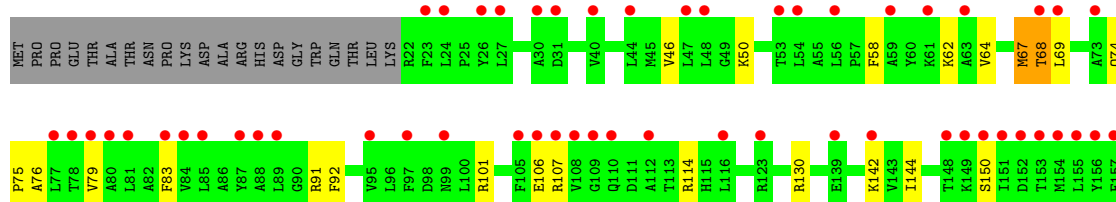
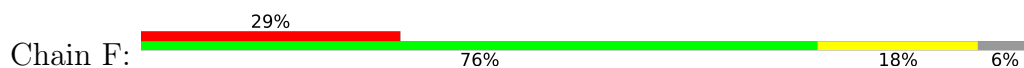


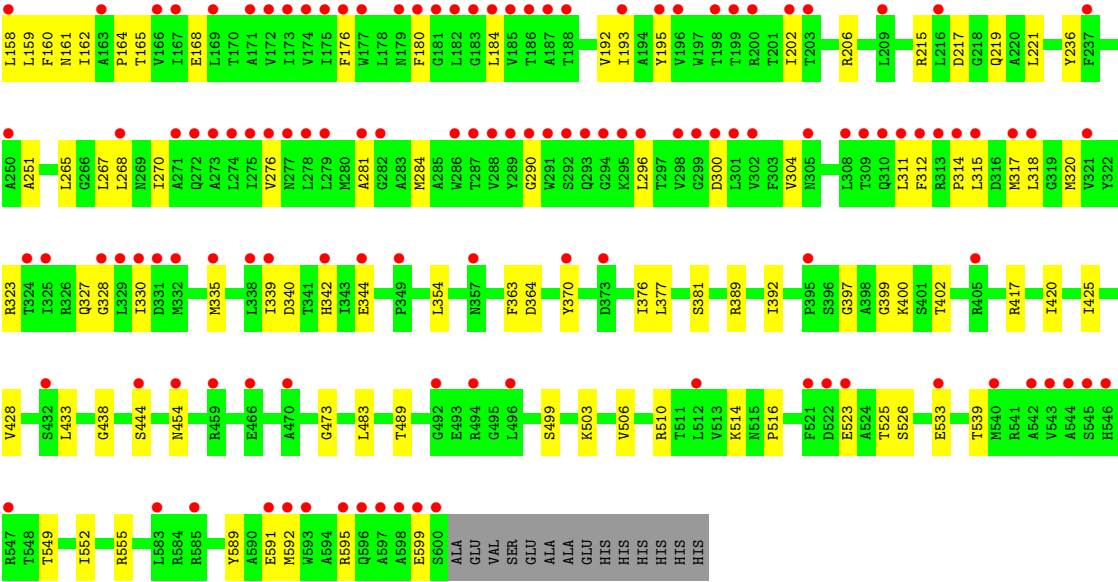


• Molecule 1: ATM1-type heavy metal exporter



• Molecule 1: ATM1-type heavy metal exporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	169.65Å 92.50Å 237.69Å 90.00° 110.34° 90.00°	Depositor
Resolution (Å)	39.62 – 3.35 39.62 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.62-3.35) 97.9 (39.62-3.35)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, REFMAC	Depositor
R, R_{free}	0.254 , 0.282 0.252 , 0.277	Depositor DCC
R_{free} test set	4901 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	26975	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: MG, ANP

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	0.15	0/4571	0.36	0/6209
1	B	0.14	0/4626	0.37	1/6284 (0.0%)
1	C	0.14	0/4523	0.36	0/6144
1	D	0.15	0/4517	0.37	0/6135
1	E	0.14	0/4452	0.34	0/6044
1	F	0.16	0/4577	0.38	0/6217
All	All	0.15	0/27266	0.36	1/37033 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	VAL	N-CA-C	-5.66	105.91	112.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4489	0	4575	60	0
1	B	4542	0	4629	81	0
1	C	4443	0	4529	96	0
1	D	4438	0	4520	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4376	0	4472	92	0
1	F	4495	0	4580	86	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
2	C	31	0	13	4	0
2	D	31	0	13	2	0
2	E	31	0	13	6	0
2	F	31	0	13	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	26975	0	27383	456	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 (456) 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:E:88:ALA:HB2	1:F:281:ALA:HB2	1.46	0.97
1:C:363:PHE:O	1:C:381:SER:HA	1.79	0.83
1:A:363:PHE:O	1:A:381:SER:HA	1.78	0.83
1:F:354:LEU:HB2	1:F:428:VAL:HG11	1.61	0.82
1:F:363:PHE:O	1:F:381:SER:HA	1.79	0.82
1:D:363:PHE:O	1:D:381:SER:HA	1.80	0.82
1:E:363:PHE:O	1:E:381:SER:HA	1.80	0.82
1:A:202:ILE:HG21	1:A:268:LEU:HB2	1.62	0.81
1:C:58:PHE:HE2	1:C:83:PHE:HA	1.46	0.80
1:D:287:THR:HG21	1:D:304:VAL:HG21	1.64	0.79
1:C:476:ILE:HG22	1:C:480:ILE:HG13	1.65	0.79
1:E:202:ILE:HG21	1:E:268:LEU:HB2	1.65	0.79
1:D:202:ILE:HG21	1:D:268:LEU:HB2	1.64	0.78
1:B:363:PHE:O	1:B:381:SER:HA	1.84	0.78
1:C:202:ILE:HG21	1:C:268:LEU:HB2	1.67	0.77
1:F:67:MET:HG3	1:F:68:THR:H	1.50	0.76
1:C:154:MET:HG2	1:C:325:ILE:HD13	1.68	0.76
1:E:268:LEU:HD23	1:E:323:ARG:HH11	1.51	0.75
1:F:397:GLY:H	2:F:701:ANP:HNB1	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:MET:HE2	1:C:298:VAL:HG21	1.70	0.73
1:E:593:TRP:HZ2	1:F:599:GLU:HG2	1.52	0.73
1:C:58:PHE:CE2	1:C:83:PHE:HA	2.24	0.71
1:F:62:LYS:HD2	1:F:79:VAL:HG22	1.73	0.70
1:F:130:ARG:NH1	1:F:344:GLU:OE2	2.24	0.70
1:A:37:ARG:NH2	1:D:32:ASN:OD1	2.26	0.69
1:B:439:ILE:HG22	1:B:520:LEU:HB3	1.75	0.69
1:D:50:LYS:CE	1:D:164:PRO:HA	2.23	0.69
1:D:56:LEU:HD13	1:D:307:TYR:HB3	1.73	0.69
1:C:280:MET:HE2	1:D:87:TYR:HE1	1.56	0.68
1:C:284:MET:HE2	1:D:83:PHE:HZ	1.58	0.68
1:E:130:ARG:NH2	1:E:370:TYR:O	2.27	0.68
1:A:165:THR:HG21	1:A:318:LEU:HG	1.74	0.68
1:D:364:ASP:OD2	1:D:417:ARG:NH2	2.27	0.68
1:F:130:ARG:NH2	1:F:370:TYR:O	2.27	0.67
1:C:35:LEU:HD22	1:C:108:VAL:HG22	1.77	0.66
1:F:150:SER:HB3	1:F:328:GLY:HA2	1.78	0.66
1:E:67:MET:SD	1:E:297:THR:OG1	2.53	0.66
1:E:130:ARG:NH1	1:E:344:GLU:OE2	2.27	0.66
1:F:420:ILE:HG13	1:F:425:ILE:HD11	1.77	0.66
1:C:161:ASN:ND2	1:C:317:MET:SD	2.69	0.66
1:A:79:VAL:O	1:A:83:PHE:HB3	1.95	0.65
1:B:62:LYS:HD2	1:B:82:ALA:HB1	1.78	0.65
1:A:130:ARG:NH2	1:A:370:TYR:O	2.30	0.65
1:C:476:ILE:HD11	1:C:505:ARG:HB2	1.79	0.64
1:E:402:THR:N	2:E:701:ANP:O2A	2.31	0.64
1:A:287:THR:HG21	1:A:304:VAL:HG21	1.79	0.64
1:D:142:LYS:HB2	1:D:221:LEU:HD23	1.78	0.63
1:B:290:GLY:HA3	1:B:296:LEU:HD13	1.79	0.63
1:C:299:GLY:O	1:C:303:PHE:HB2	1.99	0.63
1:F:79:VAL:O	1:F:83:PHE:HB3	1.99	0.62
1:C:284:MET:HE2	1:D:83:PHE:CZ	2.33	0.62
1:D:48:LEU:HD11	1:D:97:PHE:CE2	2.34	0.62
1:C:62:LYS:HD2	1:C:83:PHE:CG	2.34	0.62
1:B:202:ILE:HG21	1:B:268:LEU:HB2	1.80	0.62
1:E:142:LYS:HB2	1:E:221:LEU:HD23	1.81	0.62
1:E:74:GLN:HB3	1:E:77:LEU:HB3	1.80	0.62
1:C:67:MET:HG3	1:C:298:VAL:HG11	1.82	0.62
1:E:389:ARG:HG3	1:E:549:THR:HB	1.82	0.61
1:E:60:TYR:HB2	1:E:303:PHE:HB2	1.82	0.61
1:E:420:ILE:HG13	1:E:425:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:VAL:HG13	1:F:69:LEU:HD23	1.82	0.61
1:D:50:LYS:HE2	1:D:164:PRO:HA	1.81	0.61
1:B:523:GLU:HG3	1:B:526:SER:HB3	1.83	0.61
1:C:285:ALA:HB2	1:D:84:VAL:HG21	1.83	0.61
1:D:483:LEU:HD13	1:D:489:THR:HG21	1.82	0.61
1:C:46:VAL:HG11	1:C:164:PRO:HG3	1.83	0.60
1:C:62:LYS:HG3	1:C:79:VAL:HG13	1.83	0.60
1:F:46:VAL:HG11	1:F:164:PRO:HG3	1.83	0.60
1:D:300:ASP:O	1:D:304:VAL:HG23	2.02	0.60
1:D:420:ILE:HG13	1:D:425:ILE:HD11	1.84	0.59
2:E:701:ANP:H5'2	1:F:499:SER:HB3	1.83	0.59
1:B:335:MET:O	1:B:339:ILE:HG12	2.03	0.59
1:D:50:LYS:NZ	1:D:164:PRO:HA	2.18	0.59
1:E:354:LEU:HB2	1:E:428:VAL:HG11	1.85	0.59
1:A:150:SER:HB3	1:A:328:GLY:HA2	1.85	0.59
1:C:57:PRO:O	1:C:60:TYR:HB3	2.03	0.59
1:C:65:ASP:O	1:C:70:GLY:HA2	2.02	0.58
1:A:130:ARG:NH1	1:A:344:GLU:OE2	2.30	0.58
1:B:575:GLU:OE2	1:B:588:LEU:N	2.25	0.58
1:F:335:MET:O	1:F:339:ILE:HG13	2.03	0.58
1:C:262:GLU:HB2	1:D:106:GLU:HG2	1.84	0.58
1:D:130:ARG:NH2	1:D:370:TYR:O	2.37	0.58
1:E:593:TRP:CZ2	1:F:599:GLU:HG2	2.36	0.58
1:C:130:ARG:NH1	1:C:344:GLU:OE1	2.36	0.58
1:D:304:VAL:HG22	1:D:307:TYR:OH	2.04	0.58
1:E:62:LYS:HG3	1:E:83:PHE:HB2	1.85	0.58
1:D:150:SER:HB3	1:D:328:GLY:HA2	1.86	0.58
1:B:139:GLU:HB2	1:B:222:ALA:HB2	1.85	0.57
1:A:236:TYR:CE1	1:B:439:ILE:HD11	2.40	0.57
1:D:63:ALA:O	1:D:67:MET:HB3	2.04	0.57
1:D:354:LEU:HB2	1:D:428:VAL:HG11	1.85	0.57
1:E:473:GLY:HA2	1:E:539:THR:HG21	1.87	0.57
1:E:523:GLU:HG3	1:E:526:SER:HB3	1.86	0.57
1:A:523:GLU:HG3	1:A:526:SER:HB3	1.86	0.57
1:C:56:LEU:H	1:C:57:PRO:HD2	1.68	0.57
1:F:523:GLU:HG3	1:F:526:SER:HB3	1.85	0.57
1:C:523:GLU:HG3	1:C:526:SER:HB3	1.87	0.56
1:F:438:GLY:HA3	1:F:516:PRO:HG3	1.86	0.56
1:C:114:ARG:HG3	1:D:251:ALA:HB1	1.87	0.56
1:E:439:ILE:HD11	1:F:236:TYR:CZ	2.40	0.56
1:A:364:ASP:OD2	1:A:417:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:PHE:HE2	1:F:83:PHE:HA	1.69	0.56
1:B:420:ILE:HG13	1:B:425:ILE:HD11	1.88	0.56
1:C:56:LEU:N	1:C:57:PRO:HD2	2.21	0.56
1:C:155:LEU:O	1:C:159:LEU:HG	2.05	0.56
1:D:280:MET:HE1	1:D:305:ASN:HA	1.88	0.56
1:E:200:ARG:NH2	1:E:322:TYR:OH	2.39	0.56
1:B:361:VAL:HB	1:B:384:VAL:HB	1.88	0.55
1:F:397:GLY:HA2	2:F:701:ANP:H5'1	1.88	0.55
1:E:45:MET:HB3	1:E:101:ARG:HB2	1.88	0.55
1:D:45:MET:HA	1:D:48:LEU:HD23	1.87	0.55
1:B:318:LEU:HA	1:B:321:VAL:HB	1.88	0.55
1:C:364:ASP:OD2	1:C:417:ARG:NH2	2.39	0.55
1:D:62:LYS:HZ1	1:D:79:VAL:HA	1.72	0.55
1:E:267:LEU:O	1:E:270:ILE:HG13	2.07	0.55
1:B:130:ARG:NH2	1:B:370:TYR:O	2.40	0.55
1:E:46:VAL:HG23	1:E:101:ARG:HD3	1.88	0.55
1:E:150:SER:HB3	1:E:328:GLY:HA2	1.88	0.55
1:F:101:ARG:HD2	1:F:160:PHE:CD1	2.42	0.55
1:A:85:LEU:O	1:A:89:LEU:HB2	2.06	0.55
1:E:262:GLU:HB2	1:F:106:GLU:HG2	1.89	0.54
1:A:280:MET:HE1	1:A:305:ASN:HA	1.89	0.54
1:A:284:MET:HB2	1:B:83:PHE:CE1	2.42	0.54
1:E:63:ALA:O	1:E:67:MET:HG2	2.08	0.54
1:D:50:LYS:HZ3	1:D:164:PRO:HA	1.73	0.54
1:E:399:GLY:O	1:E:402:THR:OG1	2.26	0.54
1:E:277:ASN:OD1	1:F:91:ARG:HD2	2.08	0.54
1:F:402:THR:HG23	2:F:701:ANP:O2A	2.07	0.54
1:A:30:ALA:HB1	1:A:35:LEU:HD22	1.90	0.54
1:F:591:GLU:OE2	1:F:595:ARG:NH2	2.38	0.54
1:B:355:VAL:O	1:B:423:GLN:NE2	2.41	0.53
1:C:70:GLY:HA3	1:C:75:PRO:HB3	1.90	0.53
1:C:361:VAL:HB	1:C:384:VAL:HB	1.90	0.53
1:B:142:LYS:HB2	1:B:221:LEU:HD23	1.91	0.53
1:C:382:PHE:HB3	1:C:573:LEU:HD22	1.89	0.53
1:D:290:GLY:HA3	1:D:296:LEU:HD13	1.89	0.53
1:D:389:ARG:HG3	1:D:549:THR:HB	1.90	0.53
1:E:292:SER:OG	1:F:76:ALA:HB3	2.08	0.53
1:D:100:LEU:HA	1:D:103:ILE:HG22	1.90	0.53
1:D:523:GLU:HG3	1:D:526:SER:HB3	1.90	0.53
1:D:267:LEU:O	1:D:270:ILE:HG13	2.09	0.53
1:E:202:ILE:HG13	1:E:268:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:GLY:O	1:C:52:THR:OG1	2.26	0.53
1:E:139:GLU:HB2	1:E:222:ALA:HB2	1.90	0.53
1:C:62:LYS:HD2	1:C:83:PHE:CD1	2.43	0.53
1:E:402:THR:HG23	2:E:701:ANP:O2A	2.09	0.53
1:F:192:VAL:O	1:F:195:TYR:HD2	1.92	0.53
1:D:62:LYS:NZ	1:D:79:VAL:HA	2.24	0.53
1:E:499:SER:HB3	2:F:701:ANP:H5'2	1.90	0.52
1:F:364:ASP:OD2	1:F:417:ARG:NH2	2.42	0.52
1:F:50:LYS:HE2	1:F:164:PRO:HB3	1.91	0.52
1:A:362:THR:HB	1:A:419:LEU:HB2	1.91	0.52
1:E:62:LYS:HD2	1:E:79:VAL:HG13	1.91	0.52
1:F:402:THR:N	2:F:701:ANP:O2A	2.42	0.52
1:B:62:LYS:CD	1:B:82:ALA:HB1	2.39	0.52
1:D:158:LEU:HD12	1:D:162:ILE:HG13	1.90	0.52
1:A:408:PHE:CZ	1:B:236:TYR:HA	2.45	0.52
1:F:267:LEU:O	1:F:270:ILE:HG13	2.09	0.52
1:B:295:LYS:HA	1:E:481:ALA:HA	1.92	0.52
1:C:362:THR:HB	1:C:419:LEU:HB2	1.92	0.52
1:A:267:LEU:O	1:A:270:ILE:HG13	2.09	0.52
1:E:575:GLU:OE2	1:E:588:LEU:N	2.32	0.52
1:D:575:GLU:OE2	1:D:588:LEU:N	2.30	0.51
1:E:364:ASP:OD2	1:E:417:ARG:NH2	2.43	0.51
1:E:394:GLY:O	1:E:400:LYS:NZ	2.36	0.51
1:E:172:VAL:HG11	1:E:311:LEU:HD22	1.93	0.51
1:B:354:LEU:HB2	1:B:428:VAL:HG11	1.92	0.51
1:F:195:TYR:CE2	1:F:315:LEU:HD13	2.46	0.51
1:C:216:LEU:HD13	1:C:253:ALA:HB1	1.91	0.51
1:E:64:VAL:HG22	1:E:297:THR:HG21	1.93	0.51
1:E:291:TRP:NE1	1:E:298:VAL:HG23	2.26	0.51
1:E:397:GLY:HA2	2:E:701:ANP:H5'1	1.93	0.51
1:F:473:GLY:HA2	1:F:539:THR:HG21	1.91	0.51
1:B:279:LEU:HD23	1:B:312:PHE:HE2	1.75	0.51
1:D:430:GLN:HB3	1:D:434:ARG:NH1	2.26	0.51
1:E:146:ARG:NH1	1:E:214:ASN:HB3	2.26	0.51
1:E:209:LEU:HD13	1:E:260:LYS:HB3	1.92	0.51
1:F:76:ALA:HB1	1:F:79:VAL:HB	1.93	0.51
1:C:267:LEU:O	1:C:270:ILE:HG13	2.11	0.51
1:E:320:MET:SD	1:E:324:THR:OG1	2.68	0.51
1:B:389:ARG:HG3	1:B:549:THR:HB	1.92	0.50
2:E:701:ANP:O1A	2:E:701:ANP:N3B	2.43	0.50
1:F:311:LEU:C	1:F:314:PRO:HD2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:MET:HA	1:C:287:THR:HG22	1.93	0.50
1:C:284:MET:HB3	1:D:83:PHE:HE2	1.76	0.50
1:D:148:THR:HG23	1:D:335:MET:HE1	1.93	0.50
1:D:304:VAL:HA	1:D:307:TYR:CZ	2.46	0.50
1:A:210:ARG:HD2	1:A:327:GLN:HE22	1.76	0.50
1:C:88:ALA:HB2	1:D:281:ALA:HB2	1.94	0.50
1:F:290:GLY:HA3	1:F:296:LEU:HD13	1.94	0.50
1:F:327:GLN:HA	1:F:330:ILE:HG22	1.94	0.50
1:A:106:GLU:HG2	1:B:262:GLU:HB2	1.94	0.50
1:C:444:SER:O	1:C:503:LYS:HD3	2.12	0.50
1:D:63:ALA:HB1	1:D:298:VAL:HG23	1.93	0.50
1:A:83:PHE:HZ	1:B:284:MET:SD	2.35	0.49
1:B:362:THR:HB	1:B:419:LEU:HB2	1.94	0.49
1:C:146:ARG:NH1	1:C:214:ASN:HB3	2.27	0.49
1:A:382:PHE:HB3	1:A:573:LEU:HD22	1.94	0.49
1:D:47:LEU:O	1:D:50:LYS:HB2	2.12	0.49
1:E:256:ASP:OD1	1:F:107:ARG:NH2	2.40	0.49
1:B:202:ILE:O	1:B:206:ARG:HG2	2.12	0.49
1:D:223:ARG:HD3	1:D:246:ARG:HG3	1.94	0.49
1:D:362:THR:HB	1:D:419:LEU:HB2	1.92	0.49
1:E:507:ALA:O	1:E:510:ARG:HG2	2.12	0.49
1:F:158:LEU:HA	1:F:162:ILE:HD12	1.95	0.49
1:F:399:GLY:O	1:F:402:THR:OG1	2.29	0.49
1:F:533:GLU:OE2	1:F:555:ARG:NH1	2.44	0.49
1:A:591:GLU:OE2	1:A:595:ARG:NH2	2.41	0.49
1:C:280:MET:O	1:C:284:MET:HG3	2.13	0.49
1:E:251:ALA:HB1	1:F:114:ARG:HG3	1.94	0.49
1:E:438:GLY:HA3	1:E:516:PRO:HG3	1.93	0.49
1:A:67:MET:HE3	1:B:67:MET:HG2	1.94	0.49
1:E:296:LEU:HB3	1:E:300:ASP:OD2	2.12	0.49
1:B:46:VAL:HG11	1:B:164:PRO:HG3	1.95	0.49
1:C:50:LYS:HE3	1:C:168:GLU:HG3	1.95	0.49
1:C:223:ARG:HD3	1:C:246:ARG:HG2	1.94	0.49
1:E:206:ARG:NH2	1:E:261:SER:O	2.46	0.49
1:B:33:ALA:HB3	1:B:35:LEU:HG	1.95	0.48
1:B:172:VAL:HG11	1:B:311:LEU:HD22	1.94	0.48
1:E:313:ARG:HB3	1:E:314:PRO:HD3	1.95	0.48
1:E:376:ILE:HG21	1:E:402:THR:HG21	1.94	0.48
1:D:211:GLU:HG2	1:D:330:ILE:HG12	1.95	0.48
1:F:50:LYS:HG3	1:F:168:GLU:OE2	2.13	0.48
1:B:50:LYS:HG3	1:B:168:GLU:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HB3	1:B:57:PRO:HD3	1.94	0.48
1:A:101:ARG:NH2	1:A:102:ASN:OD1	2.44	0.48
1:A:327:GLN:HA	1:A:330:ILE:HG22	1.94	0.48
1:B:119:ASN:O	1:B:123:ARG:HG2	2.13	0.48
1:C:442:GLN:NE2	2:C:701:ANP:O3G	2.44	0.48
1:E:268:LEU:HD23	1:E:323:ARG:NH1	2.24	0.48
1:F:144:ILE:HD13	1:F:335:MET:HE2	1.96	0.48
1:F:192:VAL:HG22	1:F:315:LEU:HD11	1.95	0.48
1:C:58:PHE:CE2	1:C:86:ALA:HB3	2.48	0.48
1:D:438:GLY:HA3	1:D:516:PRO:HG3	1.95	0.48
1:C:280:MET:HE2	1:D:87:TYR:CE1	2.44	0.48
1:D:79:VAL:O	1:D:83:PHE:HB3	2.14	0.48
2:E:701:ANP:N3B	1:F:499:SER:HB2	2.29	0.48
1:B:267:LEU:O	1:B:270:ILE:HG13	2.14	0.47
1:D:58:PHE:CE2	1:D:62:LYS:HD3	2.49	0.47
1:C:417:ARG:HE	1:C:419:LEU:HD21	1.80	0.47
1:F:206:ARG:HH22	1:F:265:LEU:HD13	1.79	0.47
1:A:335:MET:O	1:A:339:ILE:HG13	2.14	0.47
1:D:389:ARG:CZ	1:D:541:ARG:HE	2.27	0.47
1:B:284:MET:HE3	1:B:305:ASN:HB2	1.97	0.47
1:C:81:LEU:O	1:C:84:VAL:HG12	2.15	0.47
1:C:374:ARG:NH1	2:C:701:ANP:O3'	2.40	0.47
1:E:445:VAL:HG13	1:E:494:ARG:HG2	1.96	0.47
1:B:347:ASP:OD1	1:B:430:GLN:HG3	2.15	0.47
1:B:425:ILE:HG13	1:B:433:LEU:HD13	1.97	0.47
1:A:114:ARG:NH1	1:A:118:GLU:OE1	2.46	0.47
1:F:142:LYS:HB2	1:F:221:LEU:HD23	1.96	0.47
1:B:327:GLN:HA	1:B:330:ILE:HG22	1.95	0.46
1:C:130:ARG:NH2	1:C:370:TYR:O	2.46	0.46
1:E:39:VAL:O	1:E:42:ALA:HB3	2.16	0.46
1:B:280:MET:HE3	1:B:284:MET:SD	2.55	0.46
1:A:146:ARG:NH1	1:A:214:ASN:HB3	2.31	0.46
1:B:78:THR:O	1:B:82:ALA:HB2	2.15	0.46
1:B:276:VAL:HG22	1:B:312:PHE:CD1	2.50	0.46
1:B:589:TYR:HA	1:B:592:MET:HE3	1.98	0.46
1:D:506:VAL:O	1:D:510:ARG:HG3	2.15	0.46
1:E:593:TRP:HZ2	1:F:599:GLU:CG	2.27	0.46
1:A:277:ASN:HD22	1:B:92:PHE:HB2	1.80	0.46
1:B:437:LEU:HD23	1:B:518:ILE:HB	1.98	0.46
1:D:75:PRO:HA	1:D:78:THR:HG22	1.97	0.46
1:C:280:MET:HA	1:C:308:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:TYR:HA	1:E:592:MET:HE3	1.98	0.46
1:F:58:PHE:CE2	1:F:83:PHE:HA	2.50	0.46
1:C:206:ARG:HH11	1:C:210:ARG:HE	1.63	0.46
1:B:202:ILE:HD12	1:B:268:LEU:HA	1.98	0.46
1:C:101:ARG:NH2	1:C:102:ASN:OD1	2.49	0.46
1:C:589:TYR:HA	1:C:592:MET:HE3	1.97	0.46
1:E:42:ALA:HB1	1:E:101:ARG:HG3	1.97	0.46
1:A:494:ARG:O	1:A:503:LYS:NZ	2.49	0.46
1:B:287:THR:HA	1:B:296:LEU:HD22	1.98	0.46
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.74	0.46
1:F:165:THR:HG21	1:F:318:LEU:HD11	1.97	0.46
1:C:445:VAL:HG13	1:C:494:ARG:HG2	1.98	0.45
1:D:588:LEU:O	1:D:592:MET:HG3	2.17	0.45
1:B:506:VAL:O	1:B:510:ARG:HG3	2.16	0.45
1:C:57:PRO:HG3	1:C:307:TYR:OH	2.15	0.45
1:C:476:ILE:HG23	1:C:479:PHE:HD2	1.81	0.45
2:C:701:ANP:O1G	1:D:499:SER:HB2	2.16	0.45
1:F:370:TYR:OH	1:F:402:THR:HG22	2.17	0.45
1:A:67:MET:HG3	1:A:68:THR:N	2.32	0.45
1:A:165:THR:HG23	1:A:314:PRO:HB2	1.99	0.45
1:F:276:VAL:HG11	1:F:312:PHE:CD2	2.51	0.45
1:D:322:TYR:O	1:D:325:ILE:HG22	2.16	0.45
1:F:425:ILE:HG23	1:F:433:LEU:HD22	1.98	0.45
1:C:209:LEU:HD13	1:C:260:LYS:HB3	1.98	0.45
1:C:499:SER:HB2	2:D:701:ANP:O2G	2.17	0.45
1:E:61:LYS:HE3	1:E:62:LYS:NZ	2.32	0.45
1:C:33:ALA:HB3	1:C:35:LEU:HG	1.99	0.45
1:C:84:VAL:HG22	1:D:281:ALA:HB1	1.99	0.45
1:D:48:LEU:HD21	1:D:97:PHE:CD1	2.51	0.45
1:E:277:ASN:HD22	1:F:92:PHE:HB2	1.82	0.45
1:F:192:VAL:HA	1:F:195:TYR:CE2	2.52	0.45
1:A:454:ASN:O	1:A:510:ARG:HG2	2.17	0.45
1:B:389:ARG:NE	1:B:541:ARG:HE	2.15	0.45
1:D:159:LEU:HD22	1:D:160:PHE:CE1	2.52	0.45
1:E:67:MET:HG3	1:E:68:THR:HG23	1.98	0.44
1:C:193:ILE:HA	1:C:196:VAL:HG22	1.99	0.44
1:C:327:GLN:HA	1:C:330:ILE:HG22	2.00	0.44
1:C:442:GLN:HE22	2:C:701:ANP:PG	2.40	0.44
1:D:56:LEU:HD22	1:D:307:TYR:HA	2.00	0.44
1:E:74:GLN:CD	1:E:77:LEU:HD23	2.42	0.44
1:F:389:ARG:HG3	1:F:549:THR:HB	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:VAL:O	1:A:510:ARG:HG3	2.18	0.44
1:B:182:LEU:HA	1:B:185:VAL:HG22	1.99	0.44
1:E:119:ASN:OD1	1:E:123:ARG:NH1	2.48	0.44
1:F:202:ILE:HG21	1:F:268:LEU:HB2	1.98	0.44
1:F:506:VAL:O	1:F:510:ARG:HG3	2.17	0.44
1:A:63:ALA:O	1:A:67:MET:HG2	2.18	0.44
1:C:142:LYS:HB2	1:C:221:LEU:HD23	1.99	0.44
1:C:306:THR:O	1:C:309:THR:OG1	2.35	0.44
1:D:361:VAL:HB	1:D:384:VAL:HB	1.99	0.44
1:E:362:THR:HB	1:E:419:LEU:HB2	2.00	0.44
1:F:340:ASP:C	1:F:342:HIS:H	2.26	0.44
1:F:589:TYR:HA	1:F:592:MET:HE3	1.99	0.44
1:C:476:ILE:HG22	1:C:476:ILE:O	2.18	0.44
1:F:176:PHE:O	1:F:180:PHE:HB2	2.17	0.44
1:A:392:ILE:HB	1:A:552:ILE:HG12	2.00	0.44
1:C:45:MET:HB3	1:C:101:ARG:HB2	1.99	0.44
1:B:206:ARG:NH2	1:B:210:ARG:HB2	2.32	0.44
1:D:63:ALA:HB3	1:D:299:GLY:HA2	1.98	0.44
1:E:322:TYR:O	1:E:325:ILE:HG22	2.18	0.44
1:F:142:LYS:HE3	1:F:217:ASP:OD2	2.17	0.44
1:B:299:GLY:O	1:B:303:PHE:HB2	2.17	0.44
1:B:537:LEU:HD23	1:B:540:MET:HE2	2.00	0.44
1:C:408:PHE:CZ	1:D:236:TYR:HA	2.53	0.44
1:A:236:TYR:CD1	1:B:439:ILE:HD11	2.52	0.43
1:B:46:VAL:CG2	1:B:101:ARG:HD3	2.48	0.43
1:E:34:VAL:O	1:E:37:ARG:HB2	2.18	0.43
1:F:400:LYS:HE2	2:F:701:ANP:O2B	2.17	0.43
1:C:62:LYS:HD3	1:D:301:LEU:HD21	1.99	0.43
1:E:49:GLY:O	1:E:52:THR:OG1	2.26	0.43
1:F:376:ILE:HG21	1:F:402:THR:HG21	2.00	0.43
1:B:451:ILE:HD11	1:B:498:LEU:HD21	2.00	0.43
1:C:150:SER:HB3	1:C:328:GLY:HA2	2.00	0.43
1:C:236:TYR:HA	1:D:408:PHE:CZ	2.52	0.43
1:E:296:LEU:HD23	1:E:296:LEU:HA	1.77	0.43
1:A:64:VAL:O	1:A:68:THR:N	2.47	0.43
1:A:367:VAL:HG22	1:A:379:GLY:H	1.83	0.43
1:C:85:LEU:HD23	1:C:85:LEU:HA	1.86	0.43
1:C:449:ASP:OD1	1:C:450:THR:HG23	2.19	0.43
1:F:180:PHE:CD2	1:F:184:LEU:HD23	2.54	0.43
1:A:64:VAL:HG23	1:A:299:GLY:HA3	1.99	0.43
1:A:438:GLY:HA3	1:A:516:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:THR:HG21	1:B:93:SER:OG	2.18	0.43
1:B:208:HIS:CE1	1:B:209:LEU:HG	2.54	0.43
1:B:438:GLY:HA3	1:B:516:PRO:HG3	1.99	0.43
1:C:336:PHE:O	1:C:339:ILE:HG13	2.18	0.43
1:A:537:LEU:HD23	1:A:540:MET:HE2	2.01	0.43
1:B:130:ARG:NH1	1:B:344:GLU:OE2	2.52	0.43
1:B:389:ARG:CZ	1:B:541:ARG:HE	2.32	0.43
1:E:355:VAL:HB	1:E:423:GLN:HE22	1.82	0.43
1:B:85:LEU:O	1:B:89:LEU:HB3	2.19	0.43
1:C:263:ASN:OD1	1:D:103:ILE:HG13	2.18	0.43
1:C:399:GLY:O	1:C:403:ILE:HG13	2.19	0.43
1:C:419:LEU:HD23	1:C:424:ASP:HA	2.00	0.43
1:E:67:MET:HE3	1:E:67:MET:HB2	1.86	0.43
1:E:69:LEU:HD23	1:E:69:LEU:HA	1.85	0.43
1:E:408:PHE:CZ	1:F:236:TYR:HA	2.54	0.43
1:B:58:PHE:CD1	1:B:303:PHE:HE1	2.36	0.43
1:D:199:THR:HA	1:D:268:LEU:HD11	2.01	0.43
1:E:311:LEU:C	1:E:314:PRO:HD2	2.43	0.43
1:F:392:ILE:HB	1:F:552:ILE:HG12	2.00	0.43
1:A:280:MET:HE2	1:B:87:TYR:HE2	1.83	0.42
1:C:67:MET:HE1	1:D:67:MET:HA	2.00	0.42
1:B:276:VAL:HG13	1:B:312:PHE:CD2	2.54	0.42
1:D:367:VAL:HG22	1:D:379:GLY:H	1.84	0.42
1:B:402:THR:N	2:B:701:ANP:O2A	2.53	0.42
1:D:58:PHE:HZ	1:D:82:ALA:HB1	1.83	0.42
1:E:588:LEU:O	1:E:592:MET:HG3	2.19	0.42
1:F:376:ILE:HG22	1:F:377:LEU:HD13	2.02	0.42
1:F:444:SER:HB2	1:F:503:LYS:HD3	2.02	0.42
1:A:169:LEU:HD23	1:A:311:LEU:HD11	2.01	0.42
1:B:28:TRP:HB3	1:B:29:PRO:HD3	2.00	0.42
1:C:36:ARG:HA	1:C:39:VAL:HG12	2.01	0.42
1:F:74:GLN:HB3	1:F:75:PRO:HD2	2.00	0.42
1:A:46:VAL:CG2	1:A:101:ARG:HD3	2.49	0.42
1:B:64:VAL:HG23	1:B:299:GLY:HA3	2.00	0.42
1:C:420:ILE:HG13	1:C:425:ILE:HD11	2.02	0.42
1:D:195:TYR:CE2	1:D:272:GLN:HB3	2.54	0.42
1:D:363:PHE:CZ	1:D:403:ILE:HG23	2.54	0.42
1:E:36:ARG:HA	1:E:39:VAL:HG12	2.02	0.42
1:B:454:ASN:O	1:B:510:ARG:HG2	2.20	0.42
1:E:114:ARG:HG3	1:F:251:ALA:HB1	2.01	0.42
1:E:522:ASP:HA	1:E:552:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:GLY:N	2:F:701:ANP:HNB1	2.11	0.42
1:B:26:TYR:O	1:B:29:PRO:HD2	2.20	0.42
1:B:206:ARG:CZ	1:B:323:ARG:HE	2.32	0.42
1:A:361:VAL:HB	1:A:384:VAL:HB	2.01	0.42
1:C:85:LEU:O	1:C:89:LEU:HB2	2.20	0.42
1:C:251:ALA:HB1	1:D:114:ARG:HG3	2.01	0.42
1:C:424:ASP:O	1:C:428:VAL:HG23	2.19	0.42
1:D:206:ARG:NH2	1:D:265:LEU:HB2	2.35	0.42
1:F:159:LEU:HD22	1:F:160:PHE:CZ	2.55	0.42
1:E:83:PHE:CE2	1:F:284:MET:HB2	2.54	0.42
1:E:425:ILE:HG23	1:E:433:LEU:HD22	2.02	0.42
1:C:389:ARG:HG3	1:C:549:THR:HB	2.02	0.41
1:E:541:ARG:NH2	1:E:561:ASP:OD2	2.53	0.41
1:F:195:TYR:CZ	1:F:315:LEU:HD13	2.56	0.41
1:B:199:THR:HG21	1:B:319:GLY:HA2	2.01	0.41
1:B:291:TRP:HA	1:B:296:LEU:O	2.20	0.41
1:C:79:VAL:HG12	1:D:288:VAL:HG21	2.03	0.41
1:D:392:ILE:HB	1:D:552:ILE:HG12	2.02	0.41
1:D:554:HIS:HE1	2:D:701:ANP:O1G	2.03	0.41
1:E:236:TYR:O	1:F:514:LYS:NZ	2.51	0.41
1:A:485:GLN:HB2	1:A:489:THR:HG22	2.02	0.41
1:B:180:PHE:HD1	1:B:286:TRP:HZ3	1.67	0.41
1:C:367:VAL:HG22	1:C:379:GLY:H	1.86	0.41
1:E:62:LYS:HD3	1:E:62:LYS:HA	1.81	0.41
1:E:370:TYR:OH	1:E:402:THR:HG22	2.21	0.41
1:E:437:LEU:HD23	1:E:518:ILE:HB	2.02	0.41
1:A:376:ILE:HG22	1:A:377:LEU:HD13	2.02	0.41
1:B:57:PRO:HB3	1:B:306:THR:HB	2.03	0.41
1:D:62:LYS:CE	1:D:79:VAL:HA	2.51	0.41
1:D:485:GLN:HB2	1:D:489:THR:CG2	2.51	0.41
1:A:291:TRP:HD1	1:A:297:THR:HA	1.85	0.41
1:E:52:THR:HG21	1:E:93:SER:OG	2.21	0.41
1:F:300:ASP:O	1:F:304:VAL:HG23	2.20	0.41
1:F:525:THR:O	1:F:555:ARG:NH1	2.53	0.41
1:A:202:ILE:HB	1:A:268:LEU:HD13	2.03	0.41
1:B:280:MET:HE1	1:B:305:ASN:HA	2.03	0.41
1:B:533:GLU:OE2	1:B:555:ARG:NH1	2.52	0.41
1:B:419:LEU:HD23	1:B:424:ASP:HA	2.03	0.41
1:D:282:GLY:O	1:D:286:TRP:CD1	2.74	0.41
1:E:177:TRP:CZ3	1:E:182:LEU:HD21	2.55	0.41
1:A:223:ARG:HD3	1:A:246:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD23	1:A:518:ILE:HB	2.03	0.41
1:C:182:LEU:HA	1:C:185:VAL:HG22	2.03	0.41
1:C:288:VAL:HG21	1:D:79:VAL:CG1	2.50	0.41
1:F:215:ARG:O	1:F:219:GLN:HG3	2.20	0.41
1:F:454:ASN:O	1:F:510:ARG:HG2	2.21	0.41
1:F:483:LEU:HD13	1:F:489:THR:HG21	2.03	0.41
1:B:195:TYR:CE1	1:B:315:LEU:HB3	2.56	0.41
1:C:227:SER:OG	1:C:243:GLU:OE1	2.35	0.41
1:C:280:MET:HG3	1:C:284:MET:SD	2.61	0.41
1:C:376:ILE:HG22	1:C:377:LEU:HD13	2.03	0.41
1:E:439:ILE:HA	1:E:520:LEU:O	2.21	0.41
1:F:320:MET:HA	1:F:323:ARG:NH2	2.36	0.41
1:A:285:ALA:N	1:B:83:PHE:HZ	2.19	0.40
1:A:367:VAL:HG22	1:A:379:GLY:N	2.37	0.40
1:C:438:GLY:HA3	1:C:516:PRO:HG3	2.03	0.40
1:D:537:LEU:HD23	1:D:540:MET:HE2	2.03	0.40
1:E:280:MET:HE3	1:E:284:MET:SD	2.62	0.40
1:A:311:LEU:C	1:A:314:PRO:HD2	2.47	0.40
1:A:445:VAL:HG13	1:A:494:ARG:HG2	2.02	0.40
1:C:354:LEU:HB2	1:C:428:VAL:HG11	2.02	0.40
1:F:161:ASN:ND2	1:F:317:MET:SD	2.95	0.40
1:E:216:LEU:HD13	1:E:253:ALA:HB1	2.03	0.40
1:A:291:TRP:HH2	1:B:71:GLY:H	1.69	0.40
1:A:363:PHE:CZ	1:A:403:ILE:HG23	2.57	0.40
1:D:376:ILE:HG22	1:D:377:LEU:HD13	2.03	0.40
1:D:494:ARG:O	1:D:503:LYS:NZ	2.55	0.40
1:E:419:LEU:HD23	1:E:424:ASP:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	576/614 (94%)	558 (97%)	18 (3%)	0	100	100
1	B	582/614 (95%)	571 (98%)	11 (2%)	0	100	100
1	C	571/614 (93%)	554 (97%)	16 (3%)	1 (0%)	43	70
1	D	571/614 (93%)	562 (98%)	9 (2%)	0	100	100
1	E	563/614 (92%)	545 (97%)	18 (3%)	0	100	100
1	F	577/614 (94%)	559 (97%)	17 (3%)	1 (0%)	43	70
All	All	3440/3684 (93%)	3349 (97%)	89 (3%)	2 (0%)	48	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	70	GLY
1	F	67	MET

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	461/491 (94%)	459 (100%)	2 (0%)	84	82
1	B	467/491 (95%)	465 (100%)	2 (0%)	84	82
1	C	456/491 (93%)	454 (100%)	2 (0%)	84	82
1	D	456/491 (93%)	449 (98%)	7 (2%)	57	68
1	E	450/491 (92%)	449 (100%)	1 (0%)	87	85
1	F	462/491 (94%)	460 (100%)	2 (0%)	84	82
All	All	2752/2946 (93%)	2736 (99%)	16 (1%)	78	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	193	ILE
1	B	67	MET

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Mol	Chain	Res	Type
1	B	172	VAL
1	C	450	THR
1	C	494	ARG
1	D	48	LEU
1	D	67	MET
1	D	172	VAL
1	D	193	ILE
1	D	263	ASN
1	D	297	THR
1	D	307	TYR
1	E	52	THR
1	F	68	THR
1	F	193	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	HIS
1	B	161	ASN
1	B	208	HIS
1	B	214	ASN
1	C	269	ASN
1	C	546	HIS
1	D	214	ASN
1	D	219	GLN
1	D	293	GLN
1	D	327	GLN
1	D	350	ASN
1	E	99	ASN
1	E	132	HIS
1	E	219	GLN
1	E	269	ASN
1	E	293	GLN
1	E	423	GLN
1	F	161	ASN
1	F	423	GLN
1	F	534	GLN

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 6 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$
2	ANP	D	701	3	33,33,33	0.88	4 (12%)	45,52,52	0.72	1 (2%)
2	ANP	E	701	3	33,33,33	0.92	4 (12%)	45,52,52	0.72	1 (2%)
2	ANP	F	701	3	33,33,33	0.95	4 (12%)	45,52,52	0.76	1 (2%)
2	ANP	B	701	3	33,33,33	0.94	4 (12%)	45,52,52	0.60	1 (2%)
2	ANP	C	701	3	33,33,33	0.84	2 (6%)	45,52,52	0.76	2 (4%)
2	ANP	A	701	3	33,33,33	0.93	4 (12%)	45,52,52	0.77	2 (4%)

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	ANP	D	701	3	-	4/18/38/38	0/3/3/3
2	ANP	E	701	3	-	6/18/38/38	0/3/3/3
2	ANP	F	701	3	-	3/18/38/38	0/3/3/3
2	ANP	B	701	3	-	4/18/38/38	0/3/3/3
2	ANP	C	701	3	-	5/18/38/38	0/3/3/3
2	ANP	A	701	3	-	1/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ANP	PG-N3B	2.72	1.70	1.63
2	E	701	ANP	PG-N3B	2.68	1.70	1.63
2	A	701	ANP	PG-O1G	2.65	1.50	1.46
2	A	701	ANP	PG-N3B	2.64	1.70	1.63
2	B	701	ANP	PG-O1G	2.57	1.50	1.46
2	F	701	ANP	PG-N3B	2.55	1.70	1.63
2	E	701	ANP	PG-O1G	2.46	1.49	1.46
2	F	701	ANP	PB-O3A	-2.38	1.56	1.59
2	C	701	ANP	PG-O1G	2.38	1.49	1.46
2	F	701	ANP	PG-O1G	2.37	1.49	1.46
2	F	701	ANP	PB-O1B	2.36	1.49	1.46
2	D	701	ANP	PG-N3B	2.35	1.69	1.63
2	C	701	ANP	PG-N3B	2.34	1.69	1.63
2	B	701	ANP	PB-O1B	2.32	1.49	1.46
2	A	701	ANP	PB-O1B	2.31	1.49	1.46
2	D	701	ANP	PG-O1G	2.28	1.49	1.46
2	D	701	ANP	PB-O1B	2.26	1.49	1.46
2	A	701	ANP	PB-N3B	2.11	1.68	1.63
2	D	701	ANP	PB-O3A	-2.07	1.56	1.59
2	E	701	ANP	PB-O3A	-2.06	1.56	1.59
2	B	701	ANP	PB-N3B	2.05	1.68	1.63
2	E	701	ANP	PB-O1B	2.03	1.49	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ANP	O3A-PB-N3B	3.43	116.11	106.59
2	F	701	ANP	O3A-PB-N3B	2.99	114.89	106.59
2	A	701	ANP	O3G-PG-O1G	-2.91	106.14	113.45
2	E	701	ANP	O1G-PG-N3B	-2.53	108.04	111.77
2	C	701	ANP	O1B-PB-N3B	-2.22	108.50	111.77
2	C	701	ANP	O3A-PB-N3B	2.16	112.58	106.59
2	D	701	ANP	O3G-PG-O1G	-2.10	108.18	113.45
2	B	701	ANP	O2G-PG-O1G	-2.08	108.23	113.45

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ANP	PB-N3B-PG-O1G
2	B	701	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	B	701	ANP	C5'-O5'-PA-O2A
2	C	701	ANP	PB-N3B-PG-O1G
2	C	701	ANP	PG-N3B-PB-O1B
2	C	701	ANP	PG-N3B-PB-O3A
2	C	701	ANP	PA-O3A-PB-O1B
2	C	701	ANP	PA-O3A-PB-O2B
2	D	701	ANP	PB-N3B-PG-O1G
2	D	701	ANP	PG-N3B-PB-O1B
2	E	701	ANP	PB-N3B-PG-O1G
2	E	701	ANP	PG-N3B-PB-O1B
2	E	701	ANP	PG-N3B-PB-O3A
2	E	701	ANP	PA-O3A-PB-O2B
2	F	701	ANP	PB-N3B-PG-O1G
2	F	701	ANP	O4'-C4'-C5'-O5'
2	F	701	ANP	C3'-C4'-C5'-O5'
2	E	701	ANP	C3'-C4'-C5'-O5'
2	B	701	ANP	C5'-O5'-PA-O1A
2	B	701	ANP	C5'-O5'-PA-O3A
2	E	701	ANP	O4'-C4'-C5'-O5'
2	D	701	ANP	PB-O3A-PA-O2A
2	D	701	ANP	PB-O3A-PA-O1A

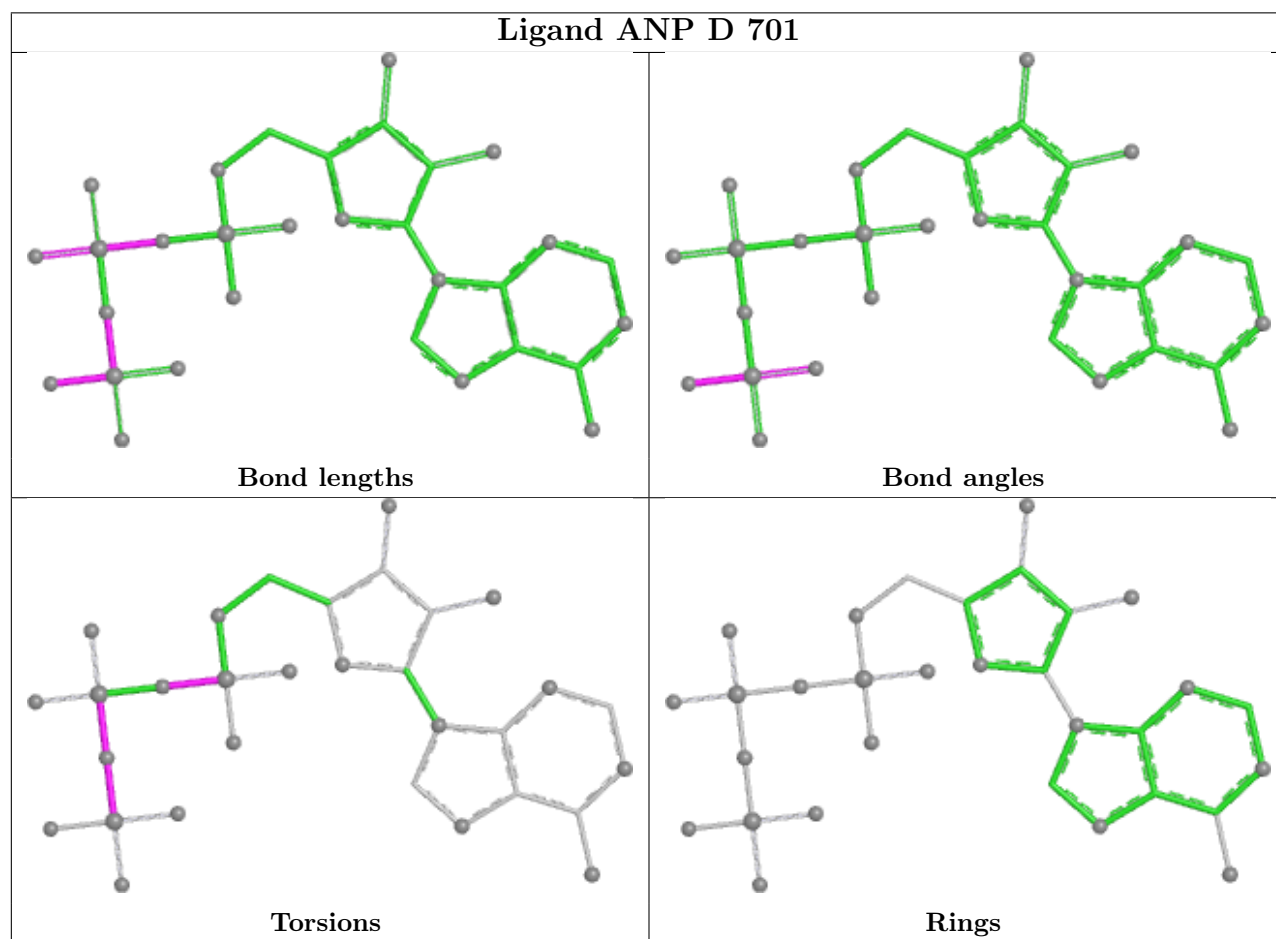
There are no ring outliers.

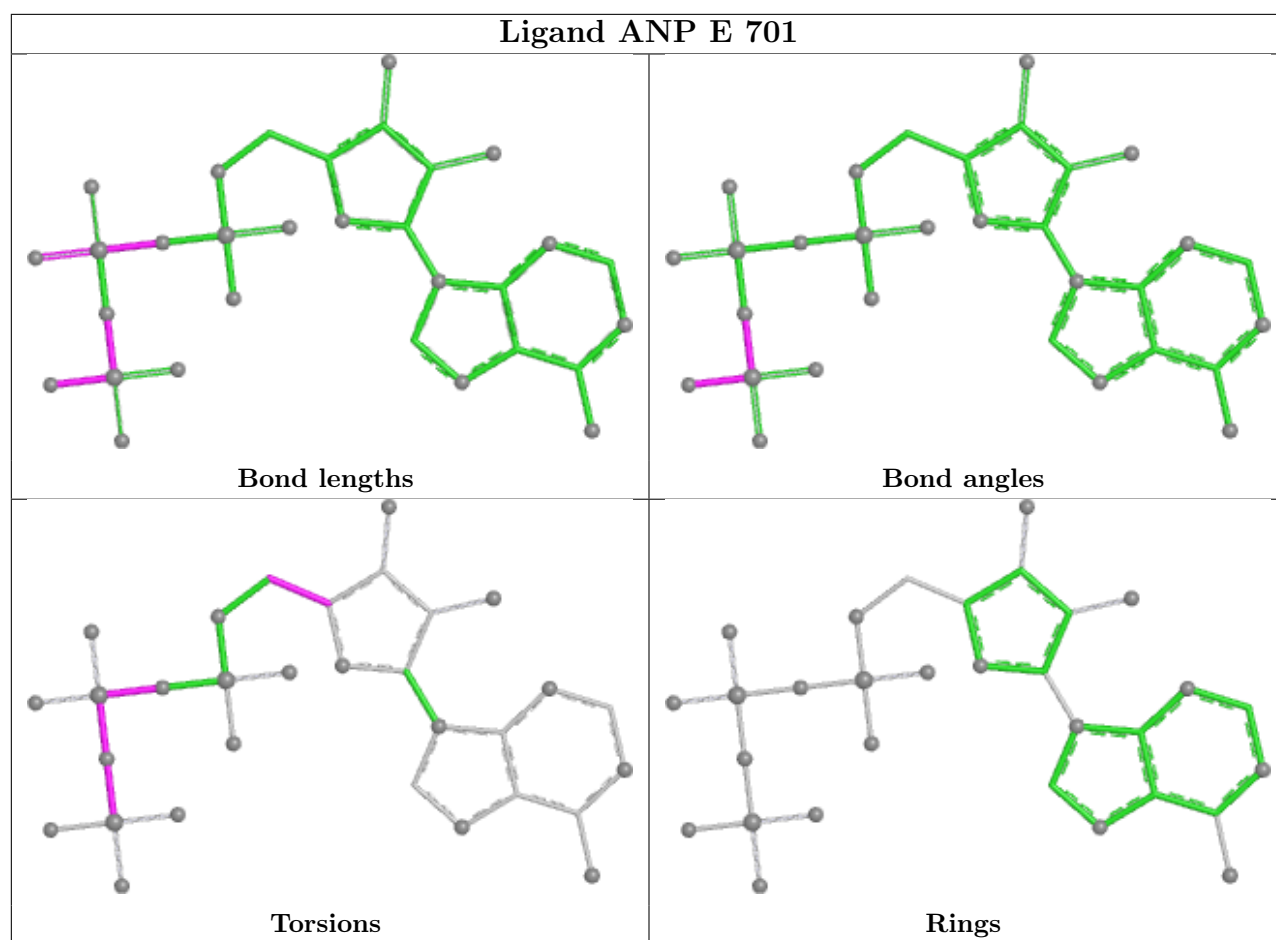
5 monomers are involved in 20 short contacts:

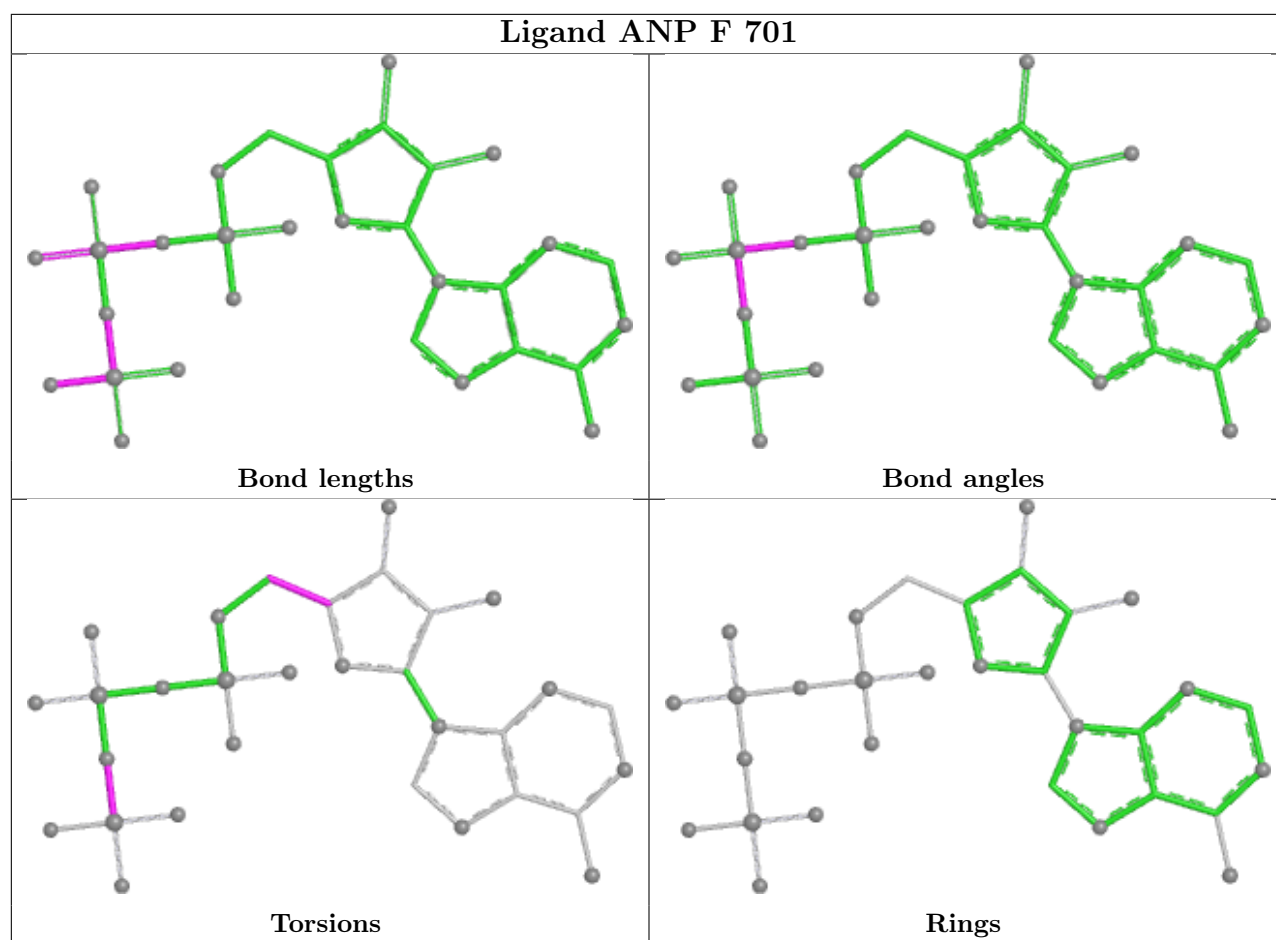
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	ANP	2	0
2	E	701	ANP	6	0
2	F	701	ANP	7	0
2	B	701	ANP	1	0
2	C	701	ANP	4	0

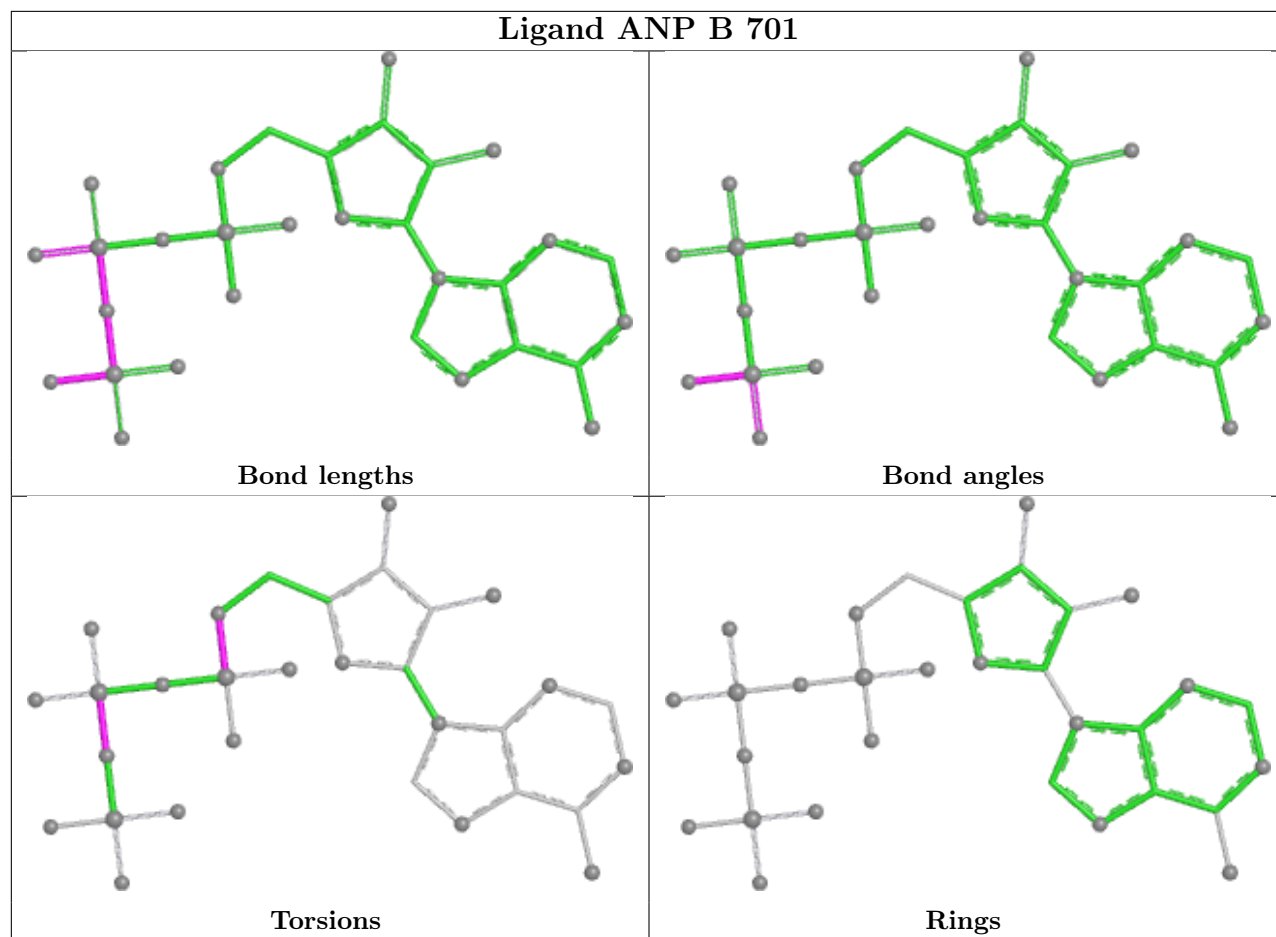
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

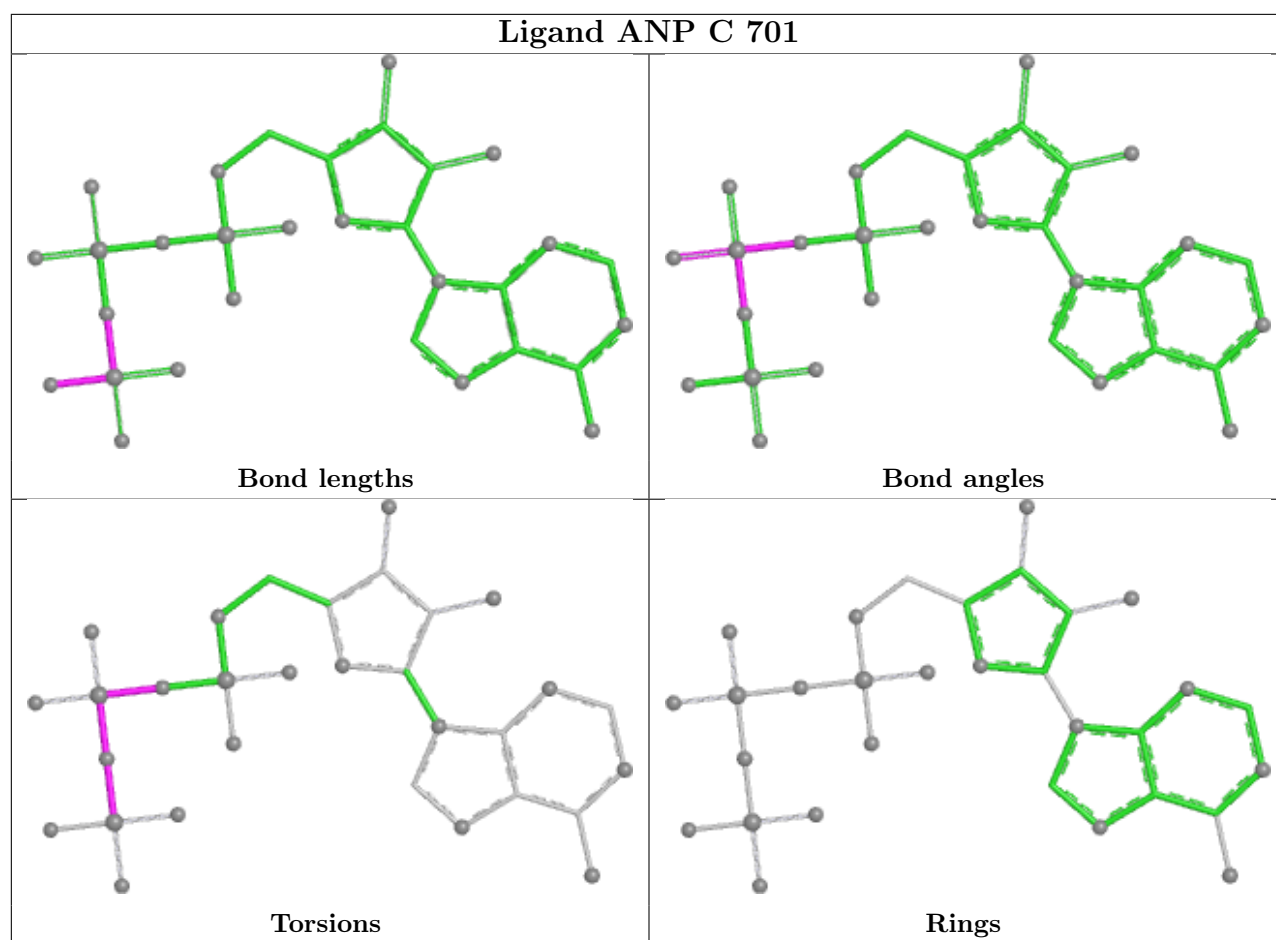
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

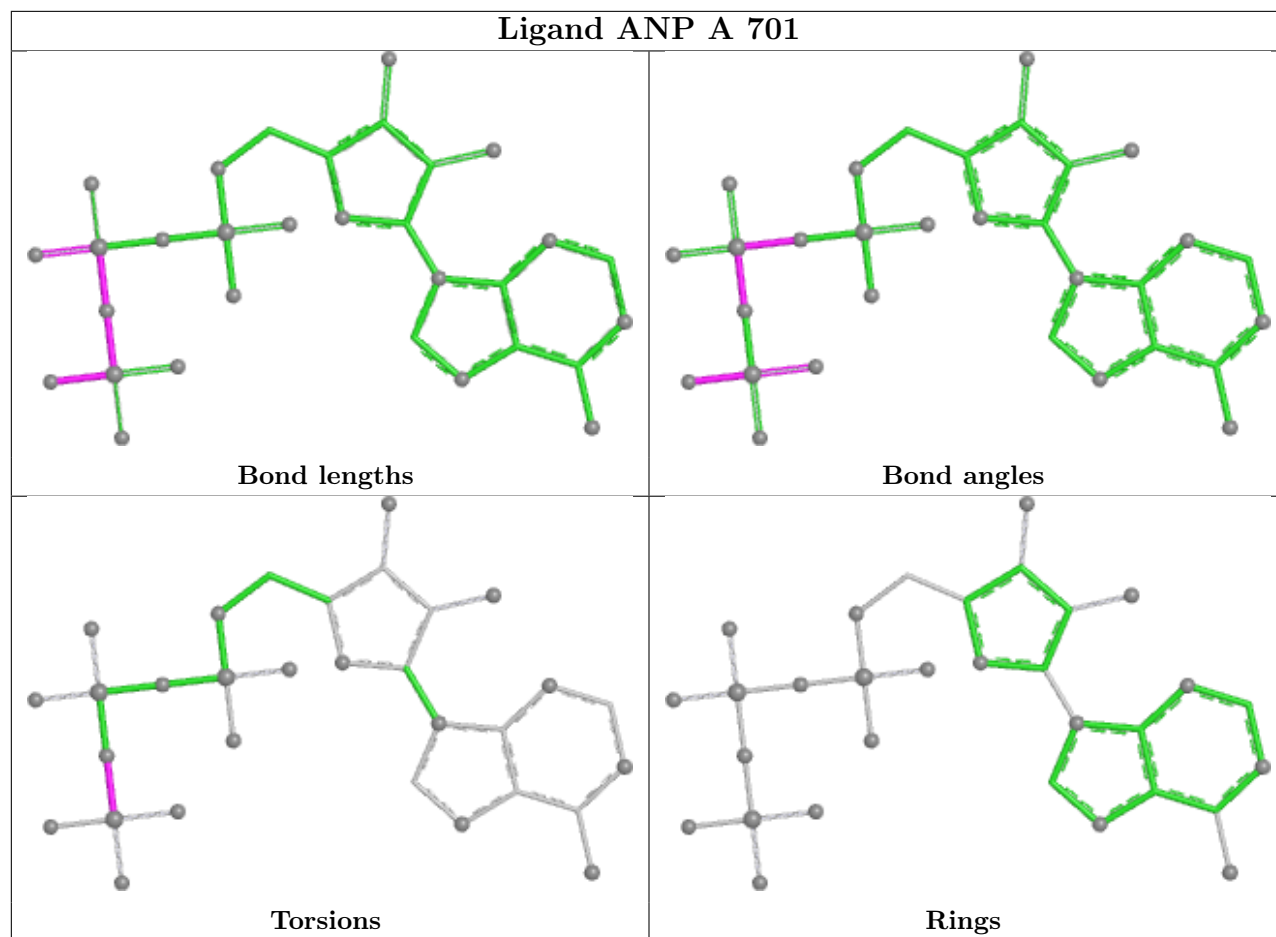












5.7 Other polymers [i](#)

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	578/614 (94%)	0.46	47 (8%)	18 15	27, 64, 123, 187	0
1	B	584/614 (95%)	0.53	56 (9%)	13 12	34, 66, 118, 181	0
1	C	573/614 (93%)	1.20	143 (24%)	2 3	87, 122, 202, 243	0
1	D	573/614 (93%)	1.60	170 (29%)	1 2	87, 127, 201, 233	0
1	E	565/614 (92%)	1.58	157 (27%)	1 2	58, 120, 304, 330	0
1	F	579/614 (94%)	1.55	178 (30%)	1 1	57, 119, 307, 346	0
All	All	3452/3684 (93%)	1.15	751 (21%)	2 4	27, 106, 262, 346	0

All (751) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	76	ALA	17.4
1	E	315	LEU	16.9
1	F	152	ASP	16.7
1	E	313	ARG	15.9
1	E	312	PHE	13.2
1	D	317	MET	12.9
1	F	328	GLY	12.7
1	D	313	ARG	12.2
1	E	316	ASP	11.4
1	F	324	THR	10.3
1	E	317	MET	10.1
1	D	316	ASP	9.6
1	B	65	ASP	9.6
1	D	98	ASP	9.5
1	E	156	TYR	9.4
1	E	195	TYR	8.7
1	F	109	GLY	8.6
1	D	320	MET	8.4
1	F	339	ILE	8.3

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Mol	Chain	Res	Type	RSRZ
1	D	598	ALA	8.2
1	E	271	ALA	8.2
1	E	98	ASP	8.2
1	C	82	ALA	8.2
1	D	153	THR	8.2
1	F	105	PHE	8.1
1	F	154	MET	8.1
1	F	153	THR	8.0
1	B	252	ARG	7.9
1	B	75	PRO	7.6
1	B	81	LEU	7.5
1	D	102	ASN	7.5
1	C	498	LEU	7.4
1	E	319	GLY	7.3
1	C	78	THR	7.3
1	B	69	LEU	7.2
1	C	353	ALA	7.1
1	E	318	LEU	7.1
1	E	59	ALA	6.8
1	E	350	ASN	6.8
1	E	50	LYS	6.7
1	F	107	ARG	6.7
1	F	357	ASN	6.7
1	B	76	ALA	6.7
1	E	154	MET	6.6
1	E	320	MET	6.6
1	E	314	PRO	6.6
1	D	321	VAL	6.6
1	D	338	LEU	6.5
1	D	131	PHE	6.4
1	C	462	ALA	6.4
1	E	311	LEU	6.4
1	D	498	LEU	6.3
1	D	157	PHE	6.3
1	C	81	LEU	6.3
1	D	80	ALA	6.3
1	F	287	THR	6.2
1	D	484	PRO	6.1
1	E	190	LEU	6.1
1	D	445	VAL	6.1
1	E	353	ALA	6.1
1	D	324	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	312	PHE	6.0
1	E	102	ASN	6.0
1	E	308	LEU	6.0
1	B	72	GLY	6.0
1	D	134	ALA	5.9
1	D	491	VAL	5.9
1	D	504	GLN	5.9
1	B	443	ASP	5.8
1	F	595	ARG	5.8
1	F	332	MET	5.8
1	F	543	VAL	5.8
1	C	352	PRO	5.8
1	F	116	LEU	5.8
1	D	443	ASP	5.7
1	B	77	LEU	5.7
1	E	56	LEU	5.7
1	C	283	ALA	5.7
1	A	443	ASP	5.7
1	D	596	GLN	5.6
1	F	335	MET	5.6
1	B	535	ASP	5.6
1	E	278	LEU	5.6
1	D	595	ARG	5.6
1	F	81	LEU	5.5
1	F	583	LEU	5.5
1	D	494	ARG	5.5
1	E	302	VAL	5.5
1	F	108	VAL	5.5
1	F	301	LEU	5.5
1	E	267	LEU	5.5
1	F	150	SER	5.5
1	F	338	LEU	5.4
1	E	535	ASP	5.4
1	E	157	PHE	5.4
1	F	522	ASP	5.3
1	C	312	PHE	5.3
1	B	73	ALA	5.3
1	D	444	SER	5.3
1	C	289	TYR	5.3
1	D	315	LEU	5.3
1	B	534	GLN	5.3
1	F	151	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	95	VAL	5.2
1	D	150	SER	5.2
1	F	288	VAL	5.1
1	E	286	TRP	5.1
1	D	28	TRP	5.0
1	E	87	TYR	5.0
1	D	446	LEU	5.0
1	F	156	TYR	5.0
1	D	312	PHE	5.0
1	E	105	PHE	5.0
1	F	286	TRP	5.0
1	C	355	VAL	4.9
1	D	55	ALA	4.9
1	D	337	ARG	4.9
1	F	155	LEU	4.9
1	E	310	GLN	4.9
1	B	256	ASP	4.9
1	F	110	GLN	4.8
1	E	192	VAL	4.8
1	C	73	ALA	4.8
1	B	85	LEU	4.8
1	F	298	VAL	4.8
1	F	599	GLU	4.8
1	C	69	LEU	4.7
1	E	160	PHE	4.7
1	F	112	ALA	4.7
1	C	71	GLY	4.7
1	C	530	THR	4.7
1	B	87	TYR	4.7
1	C	37	ARG	4.7
1	C	373	ASP	4.7
1	D	481	ALA	4.7
1	D	120	VAL	4.7
1	C	443	ASP	4.6
1	D	597	ALA	4.6
1	C	77	LEU	4.6
1	E	309	THR	4.6
1	E	321	VAL	4.6
1	A	23	PHE	4.6
1	D	193	ILE	4.5
1	D	341	THR	4.5
1	D	209	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	294	GLY	4.5
1	E	188	THR	4.4
1	D	302	VAL	4.4
1	E	276	VAL	4.4
1	F	593	TRP	4.4
1	D	492	GLY	4.4
1	D	124	LEU	4.4
1	D	59	ALA	4.4
1	E	81	LEU	4.4
1	E	149	LYS	4.4
1	F	292	SER	4.4
1	E	161	ASN	4.4
1	C	40	VAL	4.4
1	D	140	VAL	4.4
1	D	503	LYS	4.4
1	C	302	VAL	4.4
1	F	312	PHE	4.3
1	E	272	GLN	4.3
1	C	316	ASP	4.3
1	D	319	GLY	4.3
1	B	25	PRO	4.3
1	E	307	TYR	4.3
1	B	60	TYR	4.3
1	B	538	SER	4.3
1	F	302	VAL	4.3
1	A	70	GLY	4.2
1	C	34	VAL	4.2
1	C	501	GLY	4.2
1	C	301	LEU	4.2
1	E	296	LEU	4.2
1	C	68	THR	4.2
1	E	184	LEU	4.2
1	E	152	ASP	4.2
1	B	312	PHE	4.2
1	A	73	ALA	4.2
1	D	58	PHE	4.1
1	D	52	THR	4.1
1	F	349	PRO	4.1
1	E	306	THR	4.1
1	E	301	LEU	4.1
1	D	335	MET	4.1
1	D	569	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	295	LYS	4.1
1	D	74	GLN	4.1
1	D	57	PRO	4.1
1	C	495	GLY	4.1
1	E	250	ALA	4.1
1	E	283	ALA	4.1
1	E	349	PRO	4.1
1	D	56	LEU	4.0
1	D	556	LEU	4.0
1	F	23	PHE	4.0
1	F	290	GLY	4.0
1	E	53	THR	4.0
1	C	80	ALA	4.0
1	F	184	LEU	4.0
1	A	350	ASN	4.0
1	F	237	PHE	4.0
1	F	598	ALA	4.0
1	F	296	LEU	4.0
1	D	78	THR	4.0
1	F	542	ALA	4.0
1	D	310	GLN	3.9
1	D	518	ILE	3.9
1	E	275	ILE	3.9
1	D	149	LYS	3.9
1	B	24	LEU	3.9
1	F	268	LEU	3.9
1	E	150	SER	3.9
1	D	357	ASN	3.9
1	E	153	THR	3.9
1	C	598	ALA	3.9
1	D	104	VAL	3.9
1	B	309	THR	3.9
1	D	144	ILE	3.9
1	E	530	THR	3.8
1	A	69	LEU	3.8
1	E	274	LEU	3.8
1	E	101	ARG	3.8
1	F	148	THR	3.8
1	D	573	LEU	3.8
1	A	298	VAL	3.8
1	F	545	SER	3.8
1	E	180	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	287	THR	3.8
1	D	75	PRO	3.7
1	F	83	PHE	3.7
1	D	574	ALA	3.7
1	A	338	LEU	3.7
1	B	78	THR	3.7
1	E	273	ALA	3.7
1	E	598	ALA	3.7
1	B	543	VAL	3.7
1	B	67	MET	3.7
1	D	295	LYS	3.7
1	A	88	ALA	3.7
1	E	193	ILE	3.7
1	F	202	ILE	3.7
1	F	342	HIS	3.7
1	F	311	LEU	3.7
1	F	157	PHE	3.7
1	E	68	THR	3.6
1	B	66	ALA	3.6
1	D	135	ARG	3.6
1	D	287	THR	3.6
1	C	70	GLY	3.6
1	C	290	GLY	3.6
1	E	268	LEU	3.6
1	E	324	THR	3.6
1	D	336	PHE	3.6
1	D	437	LEU	3.6
1	F	444	SER	3.6
1	C	38	ARG	3.5
1	D	350	ASN	3.5
1	F	176	PHE	3.5
1	F	300	ASP	3.5
1	D	294	GLY	3.5
1	E	259	VAL	3.5
1	D	483	LEU	3.5
1	F	329	LEU	3.5
1	D	482	ARG	3.5
1	F	585	ARG	3.5
1	E	165	THR	3.5
1	B	30	ALA	3.5
1	E	281	ALA	3.5
1	C	354	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	305	ASN	3.5
1	C	293	GLN	3.5
1	C	534	GLN	3.5
1	D	79	VAL	3.5
1	E	580	LEU	3.5
1	F	330	ILE	3.5
1	E	322	TYR	3.5
1	B	79	VAL	3.5
1	D	148	THR	3.5
1	D	511	THR	3.5
1	C	149	LYS	3.4
1	E	75	PRO	3.4
1	E	365	ASN	3.4
1	F	282	GLY	3.4
1	F	186	THR	3.4
1	A	152	ASP	3.4
1	C	153	THR	3.4
1	F	310	GLN	3.4
1	F	276	VAL	3.4
1	F	308	LEU	3.4
1	F	395	PRO	3.4
1	C	269	ASN	3.3
1	E	279	LEU	3.3
1	E	280	MET	3.3
1	F	59	ALA	3.3
1	E	91	ARG	3.3
1	D	495	GLY	3.3
1	E	288	VAL	3.3
1	F	291	TRP	3.3
1	E	162	ILE	3.3
1	C	125	HIS	3.3
1	C	310	GLN	3.3
1	E	196	VAL	3.3
1	C	481	ALA	3.3
1	D	523	GLU	3.3
1	C	306	THR	3.3
1	C	327	GLN	3.3
1	C	568	LEU	3.3
1	D	205	TRP	3.3
1	C	151	ILE	3.3
1	D	591	GLU	3.3
1	D	83	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	67	MET	3.2
1	D	152	ASP	3.2
1	C	324	THR	3.2
1	F	309	THR	3.2
1	E	270	ILE	3.2
1	F	181	GLY	3.2
1	D	54	LEU	3.2
1	D	155	LEU	3.2
1	B	310	GLN	3.2
1	F	331	ASP	3.2
1	C	374	ARG	3.2
1	F	496	LEU	3.2
1	D	488	ASP	3.2
1	D	156	TYR	3.2
1	E	298	VAL	3.2
1	E	264	SER	3.2
1	E	186	THR	3.2
1	C	496	LEU	3.1
1	C	350	ASN	3.1
1	A	337	ARG	3.1
1	F	596	GLN	3.1
1	F	30	ALA	3.1
1	D	168	GLU	3.1
1	D	506	VAL	3.1
1	F	295	LYS	3.1
1	A	342	HIS	3.1
1	D	407	LEU	3.1
1	F	209	LEU	3.1
1	F	318	LEU	3.1
1	B	70	GLY	3.1
1	D	151	ILE	3.1
1	F	87	TYR	3.1
1	A	305	ASN	3.1
1	F	80	ALA	3.1
1	D	53	THR	3.1
1	E	72	GLY	3.1
1	F	492	GLY	3.1
1	C	54	LEU	3.0
1	F	272	GLN	3.0
1	C	292	SER	3.0
1	C	463	SER	3.0
1	F	106	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	139	GLU	3.0
1	D	175	ILE	3.0
1	D	289	TYR	3.0
1	C	76	ALA	3.0
1	D	496	LEU	3.0
1	D	132	HIS	3.0
1	E	579	HIS	3.0
1	F	123	ARG	3.0
1	F	196	VAL	3.0
1	C	67	MET	3.0
1	C	332	MET	3.0
1	F	466	GLU	3.0
1	A	488	ASP	3.0
1	C	318	LEU	3.0
1	E	89	LEU	3.0
1	F	31	ASP	3.0
1	F	182	LEU	3.0
1	E	73	ALA	3.0
1	F	63	ALA	3.0
1	F	546	HIS	3.0
1	E	305	ASN	3.0
1	F	293	GLN	3.0
1	E	83	PHE	3.0
1	F	97	PHE	3.0
1	F	188	THR	3.0
1	E	69	LEU	3.0
1	D	554	HIS	3.0
1	C	461	GLY	3.0
1	C	287	THR	3.0
1	F	275	ILE	3.0
1	D	480	ILE	3.0
1	D	318	LEU	2.9
1	E	541	ARG	2.9
1	B	542	ALA	2.9
1	E	142	LYS	2.9
1	D	500	GLY	2.9
1	F	174	VAL	2.9
1	C	59	ALA	2.9
1	D	192	VAL	2.9
1	E	79	VAL	2.9
1	D	438	GLY	2.9
1	D	29	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	88	ALA	2.9
1	F	600	SER	2.9
1	C	35	LEU	2.9
1	F	317	MET	2.9
1	C	297	THR	2.9
1	C	351	ALA	2.9
1	F	299	GLY	2.9
1	D	406	LEU	2.9
1	E	439	ILE	2.9
1	F	48	LEU	2.9
1	C	398	ALA	2.9
1	E	80	ALA	2.9
1	F	199	THR	2.9
1	F	250	ALA	2.9
1	F	95	VAL	2.9
1	C	87	TYR	2.9
1	D	101	ARG	2.9
1	A	339	ILE	2.9
1	C	296	LEU	2.9
1	D	420	ILE	2.9
1	C	286	TRP	2.8
1	C	494	ARG	2.8
1	D	36	ARG	2.8
1	C	178	LEU	2.8
1	C	317	MET	2.8
1	C	65	ASP	2.8
1	D	497	LYS	2.8
1	A	27	LEU	2.8
1	E	175	ILE	2.8
1	E	178	LEU	2.8
1	B	86	ALA	2.8
1	A	300	ASP	2.8
1	C	229	LEU	2.8
1	C	267	LEU	2.8
1	F	44	LEU	2.8
1	F	521	PHE	2.8
1	C	60	TYR	2.8
1	D	323	ARG	2.8
1	F	200	ARG	2.8
1	A	34	VAL	2.8
1	B	306	THR	2.8
1	A	522	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	303	PHE	2.8
1	C	307	TYR	2.8
1	E	220	ALA	2.8
1	B	260	LYS	2.8
1	D	145	GLU	2.8
1	E	284	MET	2.7
1	C	497	LYS	2.7
1	F	84	VAL	2.7
1	D	133	LEU	2.7
1	F	27	LEU	2.7
1	D	103	ILE	2.7
1	E	189	ILE	2.7
1	D	530	THR	2.7
1	C	422	GLY	2.7
1	E	438	GLY	2.7
1	C	64	VAL	2.7
1	D	288	VAL	2.7
1	E	550	ILE	2.7
1	D	592	MET	2.7
1	C	500	GLY	2.7
1	D	526	SER	2.7
1	F	149	LYS	2.7
1	C	179	ASN	2.7
1	F	73	ALA	2.7
1	C	393	VAL	2.7
1	F	166	VAL	2.7
1	D	184	LEU	2.7
1	F	85	LEU	2.7
1	F	158	LEU	2.7
1	C	576	GLN	2.7
1	A	341	THR	2.7
1	C	526	SER	2.7
1	A	65	ASP	2.7
1	E	66	ALA	2.7
1	F	274	LEU	2.7
1	C	75	PRO	2.7
1	C	303	PHE	2.7
1	A	584	ARG	2.7
1	B	541	ARG	2.7
1	A	276	VAL	2.7
1	A	301	LEU	2.7
1	C	537	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	77	LEU	2.7
1	D	95	VAL	2.7
1	D	433	LEU	2.7
1	E	115	HIS	2.7
1	D	565	ILE	2.6
1	B	523	GLU	2.6
1	E	241	SER	2.6
1	F	163	ALA	2.6
1	C	31	ASP	2.6
1	E	339	ILE	2.6
1	F	167	ILE	2.6
1	B	149	LYS	2.6
1	F	142	LYS	2.6
1	F	547	ARG	2.6
1	C	493	GLU	2.6
1	C	56	LEU	2.6
1	D	301	LEU	2.6
1	E	82	ALA	2.6
1	F	314	PRO	2.6
1	F	540	MET	2.6
1	C	74	GLN	2.6
1	B	33	ALA	2.6
1	E	148	THR	2.6
1	E	166	VAL	2.6
1	F	175	ILE	2.6
1	D	277	ASN	2.6
1	B	82	ALA	2.6
1	C	567	VAL	2.6
1	E	63	ALA	2.6
1	E	78	THR	2.6
1	F	177	TRP	2.6
1	C	58	PHE	2.6
1	D	405	ARG	2.6
1	D	297	THR	2.6
1	F	289	TYR	2.5
1	E	77	LEU	2.5
1	F	99	ASN	2.5
1	F	198	THR	2.5
1	A	24	LEU	2.5
1	C	499	SER	2.5
1	F	494	ARG	2.5
1	D	300	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	88	ALA	2.5
1	E	151	ILE	2.5
1	C	176	PHE	2.5
1	E	407	LEU	2.5
1	F	279	LEU	2.5
1	A	112	ALA	2.5
1	E	191	ALA	2.5
1	E	139	GLU	2.5
1	E	99	ASN	2.5
1	E	549	THR	2.5
1	F	180	PHE	2.5
1	F	203	THR	2.5
1	C	308	LEU	2.5
1	C	503	LYS	2.5
1	F	69	LEU	2.5
1	F	512	LEU	2.5
1	C	298	VAL	2.5
1	C	66	ALA	2.5
1	F	193	ILE	2.5
1	D	408	PHE	2.5
1	B	319	GLY	2.5
1	C	492	GLY	2.5
1	D	46	VAL	2.5
1	F	171	ALA	2.4
1	F	271	ALA	2.4
1	B	17	TRP	2.4
1	D	197	TRP	2.4
1	D	593	TRP	2.4
1	F	68	THR	2.4
1	C	288	VAL	2.4
1	D	34	VAL	2.4
1	F	172	VAL	2.4
1	F	183	GLY	2.4
1	E	76	ALA	2.4
1	F	325	ILE	2.4
1	C	145	GLU	2.4
1	C	336	PHE	2.4
1	E	338	LEU	2.4
1	E	488	ASP	2.4
1	A	59	ALA	2.4
1	A	320	MET	2.4
1	C	91	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	447	PHE	2.4
1	F	533	GLU	2.4
1	E	158	LEU	2.4
1	C	309	THR	2.4
1	F	454	ASN	2.4
1	A	394	GLY	2.4
1	F	281	ALA	2.4
1	F	544	ALA	2.4
1	A	83	PHE	2.4
1	D	286	TRP	2.4
1	C	569	ASP	2.4
1	D	90	GLY	2.4
1	A	66	ALA	2.4
1	D	334	GLU	2.4
1	A	28	TRP	2.4
1	B	259	VAL	2.4
1	E	64	VAL	2.4
1	E	532	THR	2.3
1	C	574	ALA	2.3
1	E	552	ILE	2.3
1	D	279	LEU	2.3
1	E	303	PHE	2.3
1	F	278	LEU	2.3
1	C	28	TRP	2.3
1	C	275	ILE	2.3
1	D	30	ALA	2.3
1	E	208	HIS	2.3
1	F	470	ALA	2.3
1	D	589	TYR	2.3
1	E	269	ASN	2.3
1	F	195	TYR	2.3
1	F	305	ASN	2.3
1	D	364	ASP	2.3
1	A	74	GLN	2.3
1	D	173	ILE	2.3
1	C	258	ALA	2.3
1	D	86	ALA	2.3
1	E	258	ALA	2.3
1	E	435	ALA	2.3
1	E	546	HIS	2.3
1	D	333	ALA	2.3
1	D	306	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	35	LEU	2.3
1	C	305	ASN	2.3
1	B	74	GLN	2.3
1	C	331	ASP	2.3
1	C	276	VAL	2.3
1	F	40	VAL	2.3
1	D	527	ALA	2.3
1	E	265	LEU	2.3
1	F	56	LEU	2.3
1	D	208	HIS	2.3
1	F	26	TYR	2.3
1	A	62	LYS	2.3
1	C	504	GLN	2.3
1	C	300	ASP	2.3
1	D	516	PRO	2.2
1	C	209	LEU	2.2
1	E	593	TRP	2.2
1	B	53	THR	2.2
1	F	53	THR	2.2
1	F	78	THR	2.2
1	B	62	LYS	2.2
1	D	195	TYR	2.2
1	F	61	LYS	2.2
1	B	91	ARG	2.2
1	F	405	ARG	2.2
1	C	39	VAL	2.2
1	A	244	GLU	2.2
1	F	591	GLU	2.2
1	C	392	ILE	2.2
1	E	167	ILE	2.2
1	C	30	ALA	2.2
1	F	89	LEU	2.2
1	F	273	ALA	2.2
1	D	188	THR	2.2
1	E	342	HIS	2.2
1	E	405	ARG	2.2
1	F	370	TYR	2.2
1	B	32	ASN	2.2
1	E	277	ASN	2.2
1	F	277	ASN	2.2
1	A	175	ILE	2.2
1	F	173	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	522	ASP	2.2
1	C	55	ALA	2.2
1	C	338	LEU	2.2
1	D	69	LEU	2.2
1	E	187	ALA	2.2
1	E	255	ALA	2.2
1	E	528	LEU	2.2
1	E	249	SER	2.2
1	C	85	LEU	2.2
1	D	599	GLU	2.2
1	F	216	LEU	2.2
1	F	315	LEU	2.2
1	B	29	PRO	2.2
1	B	59	ALA	2.2
1	E	88	ALA	2.2
1	E	443	ASP	2.2
1	A	78	THR	2.2
1	A	115	HIS	2.2
1	B	199	THR	2.2
1	C	341	THR	2.2
1	E	247	TYR	2.2
1	F	432	SER	2.2
1	C	155	LEU	2.2
1	F	523	GLU	2.2
1	A	142	LYS	2.2
1	C	235	LYS	2.2
1	D	33	ALA	2.2
1	D	62	LYS	2.2
1	D	142	LYS	2.2
1	D	486	GLY	2.2
1	E	61	LYS	2.2
1	E	92	PHE	2.2
1	C	491	VAL	2.1
1	C	173	ILE	2.1
1	D	189	ILE	2.1
1	C	265	LEU	2.1
1	C	381	SER	2.1
1	D	396	SER	2.1
1	C	502	GLU	2.1
1	E	465	ALA	2.1
1	B	71	GLY	2.1
1	D	49	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	185	VAL	2.1
1	C	511	THR	2.1
1	D	207	THR	2.1
1	A	335	MET	2.1
1	C	358	ARG	2.1
1	F	313	ARG	2.1
1	A	422	GLY	2.1
1	B	28	TRP	2.1
1	F	321	VAL	2.1
1	F	373	ASP	2.1
1	D	167	ILE	2.1
1	B	26	TYR	2.1
1	E	62	LYS	2.1
1	F	47	LEU	2.1
1	D	252	ARG	2.1
1	E	163	ALA	2.1
1	C	479	PHE	2.1
1	A	316	ASP	2.1
1	C	62	LYS	2.1
1	C	593	TRP	2.1
1	C	315	LEU	2.1
1	A	313	ARG	2.1
1	C	320	MET	2.1
1	F	592	MET	2.1
1	D	219	GLN	2.1
1	A	336	PHE	2.1
1	C	395	PRO	2.1
1	F	344	GLU	2.1
1	F	79	VAL	2.1
1	C	343	ILE	2.1
1	D	206	ARG	2.1
1	D	451	ILE	2.1
1	E	228	LEU	2.1
1	D	342	HIS	2.1
1	E	323	ARG	2.1
1	F	169	LEU	2.1
1	B	19	THR	2.1
1	F	187	ALA	2.1
1	B	504	GLN	2.1
1	C	182	LEU	2.0
1	D	547	ARG	2.0
1	E	531	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	572	ARG	2.0
1	F	179	ASN	2.0
1	F	459	ARG	2.0
1	A	87	TYR	2.0
1	C	421	ASP	2.0
1	F	597	ALA	2.0
1	C	473	GLY	2.0
1	C	445	VAL	2.0
1	D	229	LEU	2.0
1	E	337	ARG	2.0
1	E	556	LEU	2.0
1	F	24	LEU	2.0
1	F	54	LEU	2.0
1	F	77	LEU	2.0
1	B	335	MET	2.0
1	D	332	MET	2.0
1	A	52	THR	2.0
1	D	331	ASP	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.

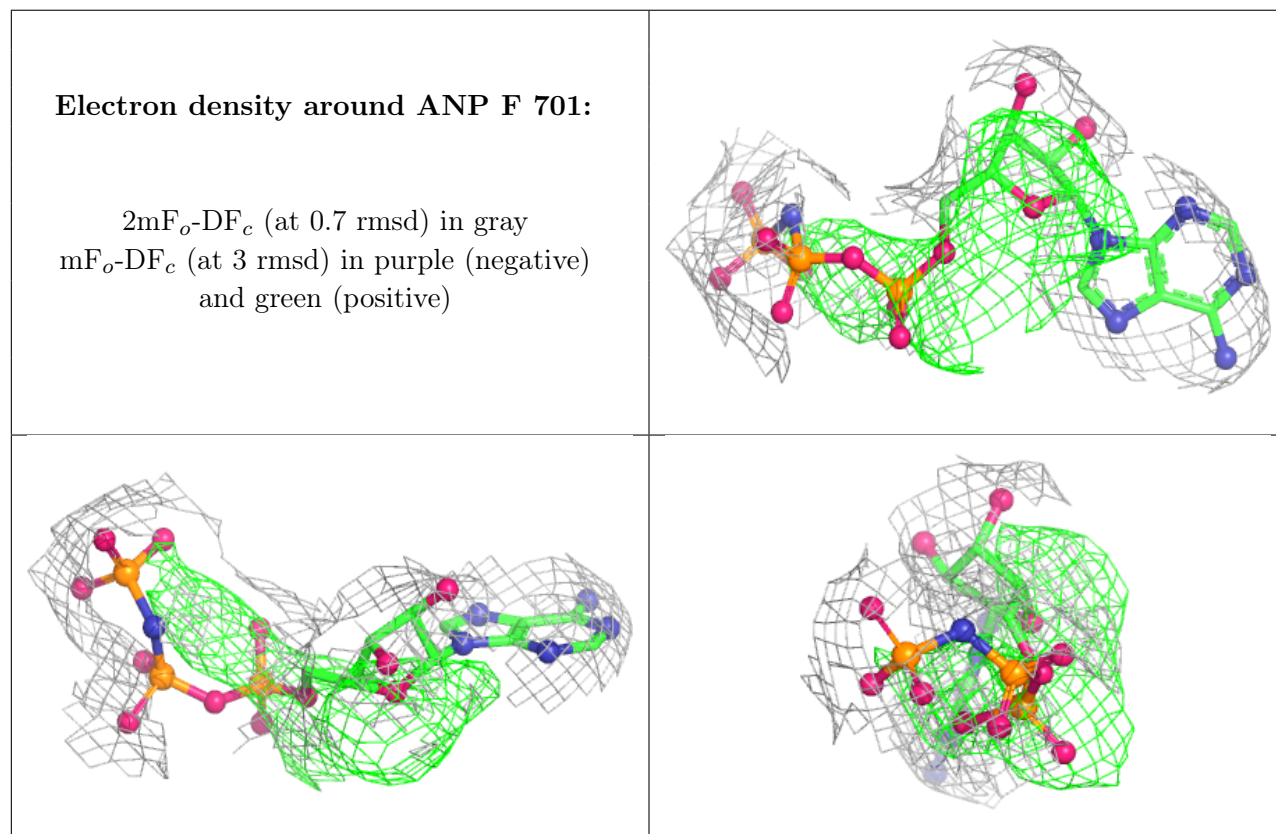
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ANP	F	701	31/31	0.90	0.18	74,98,125,129	0
3	MG	A	702	1/1	0.90	0.22	36,36,36,36	0
2	ANP	D	701	31/31	0.91	0.13	102,124,134,138	0
2	ANP	E	701	31/31	0.91	0.17	86,117,141,153	0
3	MG	D	702	1/1	0.92	0.10	87,87,87,87	0

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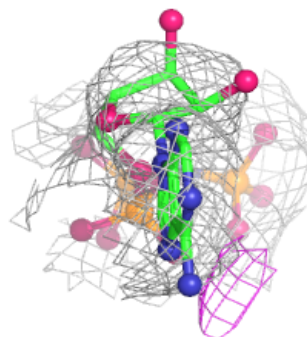
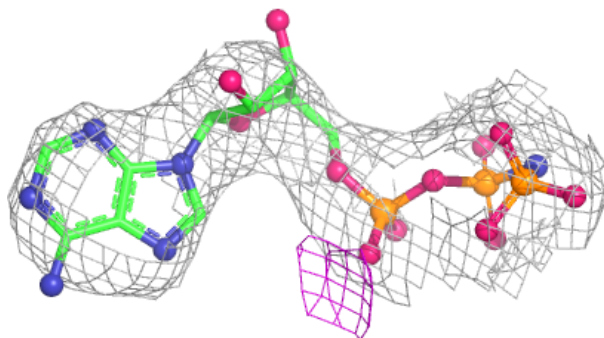
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	702	1/1	0.93	0.18	49,49,49,49	0
2	ANP	C	701	31/31	0.93	0.12	103,139,160,178	0
3	MG	E	702	1/1	0.94	0.13	52,52,52,52	0
2	ANP	A	701	31/31	0.95	0.11	38,58,83,99	0
2	ANP	B	701	31/31	0.96	0.12	40,71,82,96	0
3	MG	C	702	1/1	0.96	0.12	116,116,116,116	0
3	MG	F	702	1/1	0.97	0.12	64,64,64,64	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.

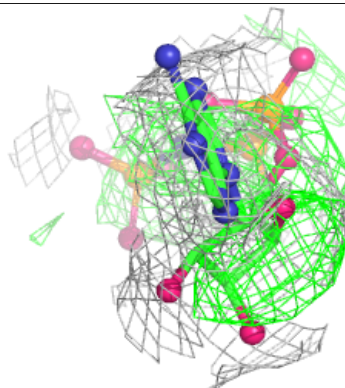
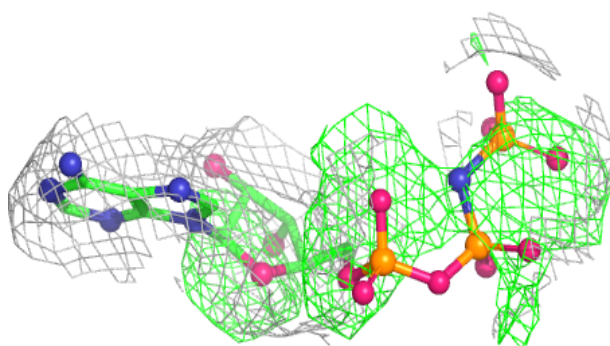
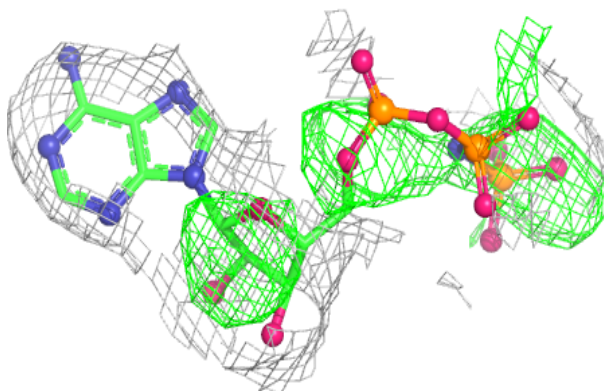


Electron density around ANP D 701:

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

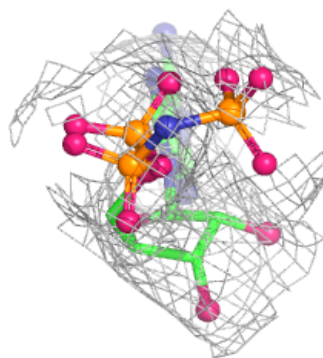
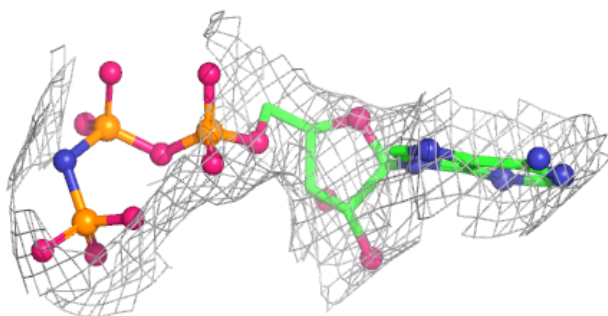
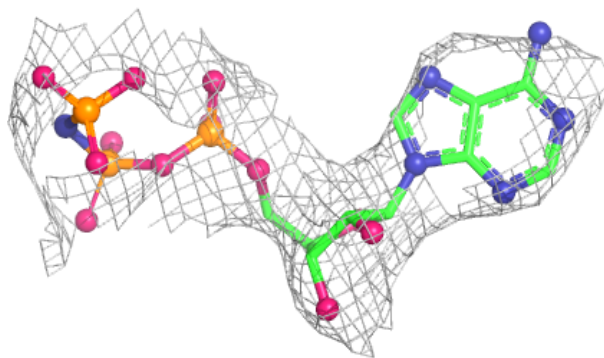
**Electron density around ANP E 701:**

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

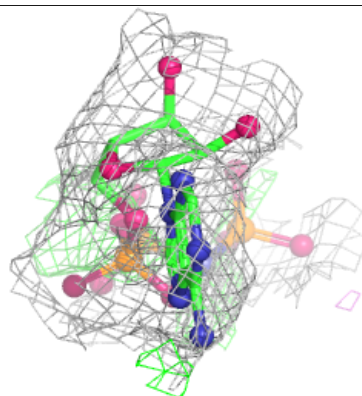
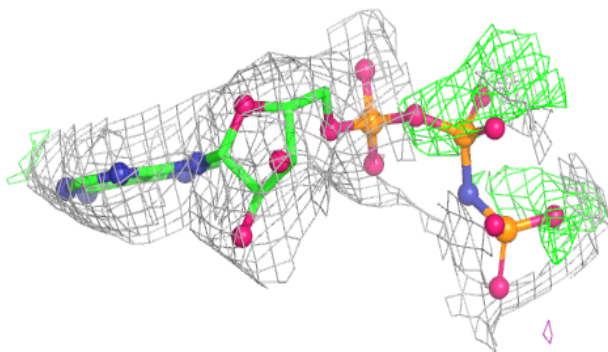
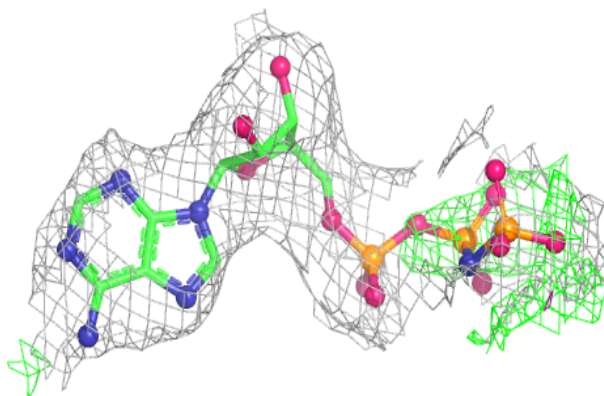


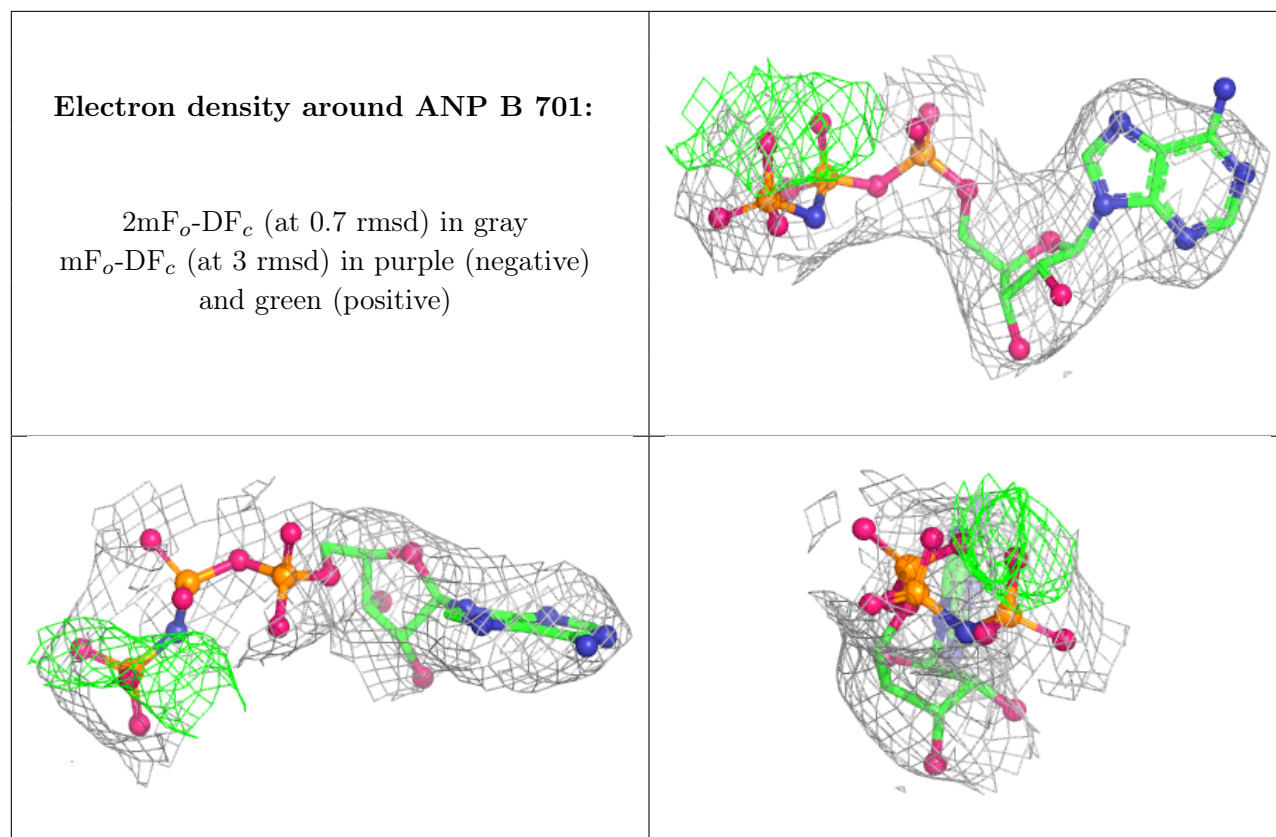
Electron density around ANP C 701:

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

**Electron density around ANP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.