



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 01:47 PM BST

PDB ID : 6PAR
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

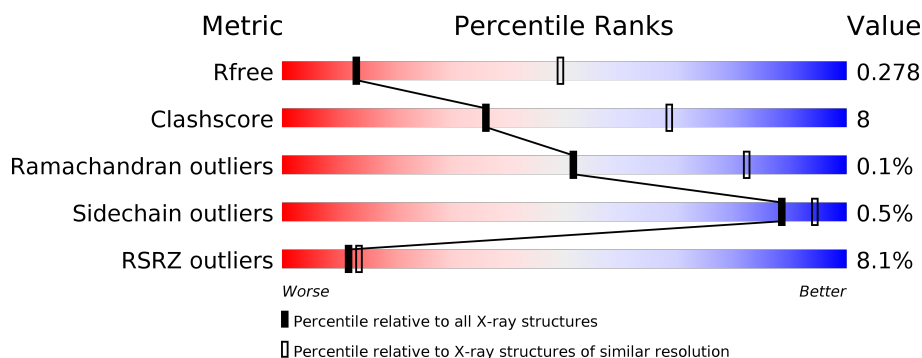
1 Overall quality at a glance

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}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
1	B	614	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>5%</div> </div> </div>
1	C	614	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>7%</div> </div> </div>
1	D	614	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>7%</div> </div> </div>
1	E	614	<div> <div>11%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>8%</div> </div> </div>
1	F	614	<div> <div>16%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>6%</div> </div> </div>

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:

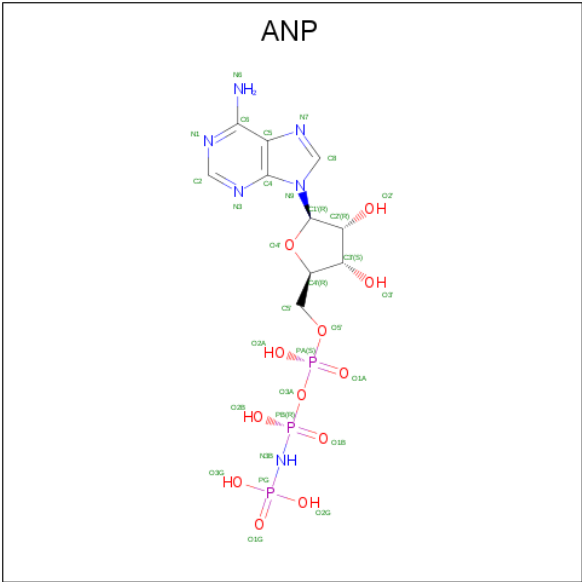
Chain	Residue	Modelled	Actual	Comment	Reference
A	609	HIS	-	expression tag	UNP Q2G506
A	610	HIS	-	expression tag	UNP Q2G506
A	611	HIS	-	expression tag	UNP Q2G506
A	612	HIS	-	expression tag	UNP Q2G506
A	613	HIS	-	expression tag	UNP Q2G506
A	614	HIS	-	expression tag	UNP Q2G506
B	609	HIS	-	expression tag	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 (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

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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		

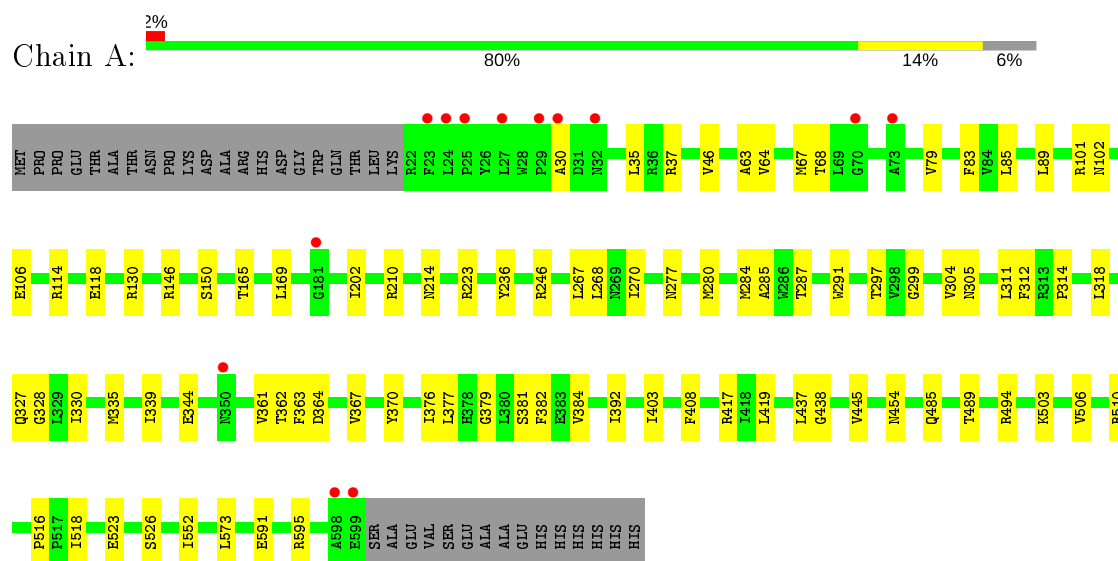
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

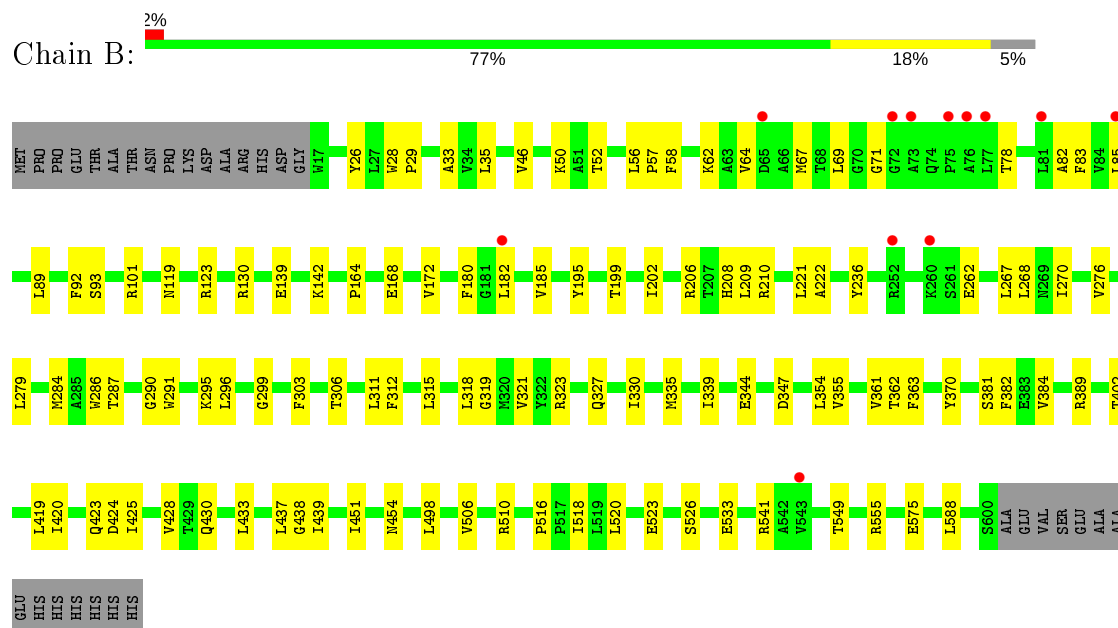
3 Residue-property plots [i](#)

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.

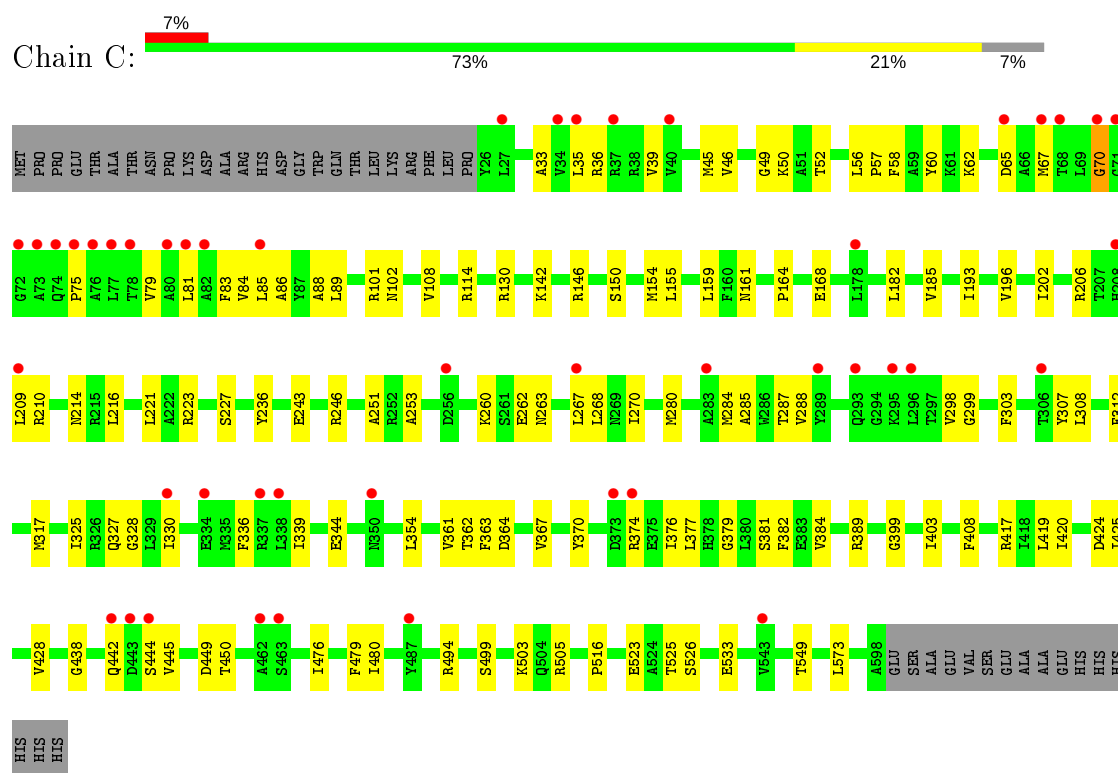
- Molecule 1: ATM1-type heavy metal exporter



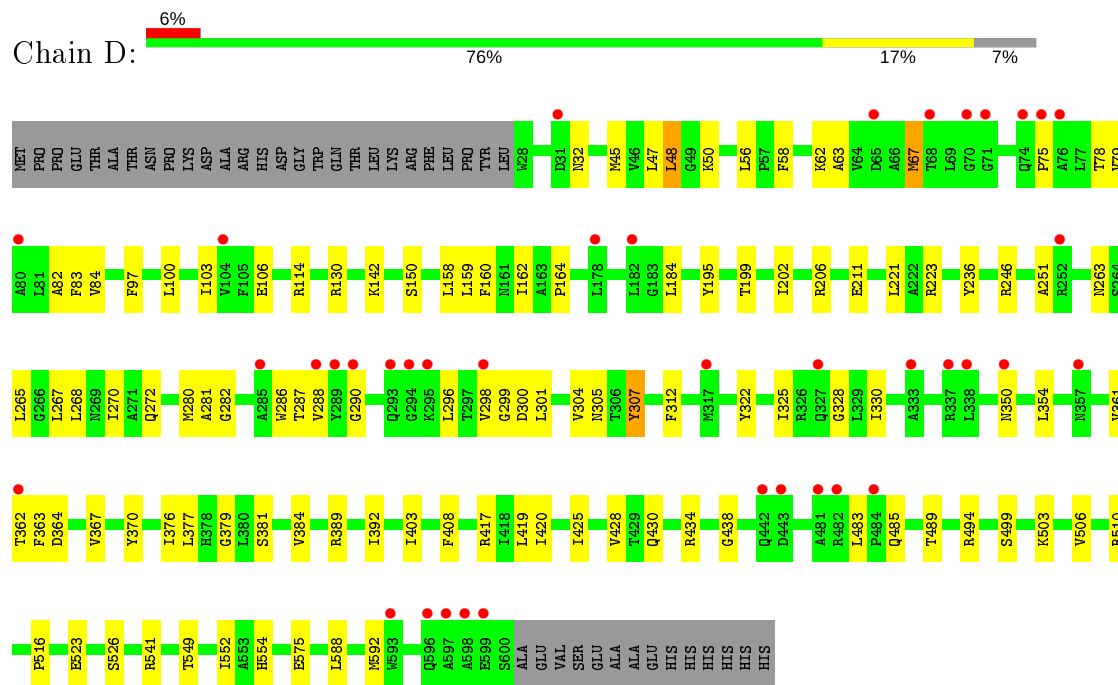
- Molecule 1: ATM1-type heavy metal exporter



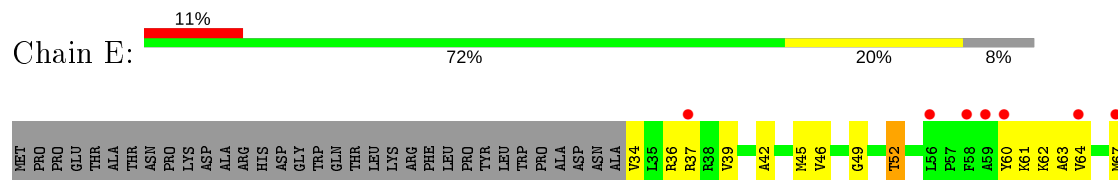
- Molecule 1: ATM1-type heavy metal exporter

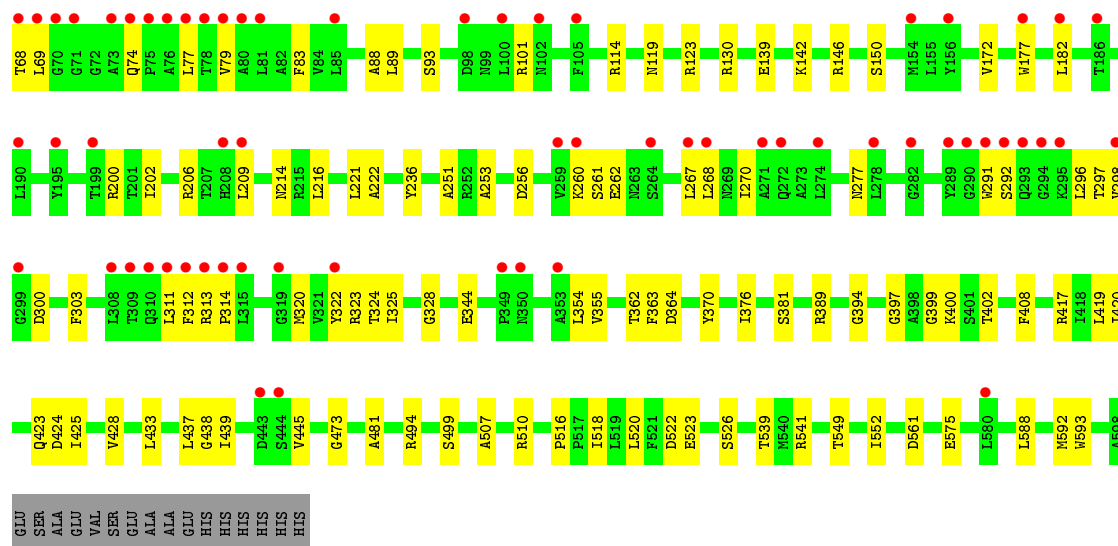


- Molecule 1: ATM1-type heavy metal exporter

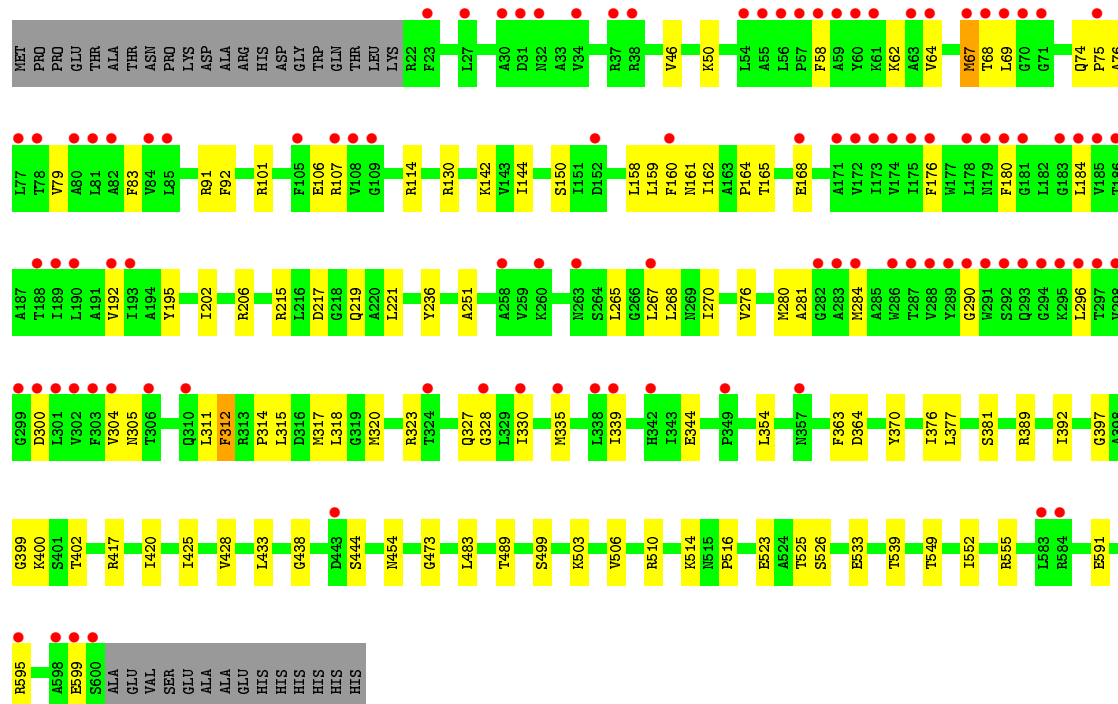


- Molecule 1: ATM1-type heavy metal exporter





● 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 39.77 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.62-3.35) 98.0 (39.77-3.35)	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 , 0.278	Depositor DCC
R_{free} test set	4901 reflections (5.00%)	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)	0.24 , 70.7	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	0.86	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	0.25	0/4571	0.43	0/6209
1	B	0.26	0/4626	0.45	0/6284
1	C	0.25	0/4523	0.44	0/6144
1	D	0.25	0/4517	0.45	0/6135
1	E	0.25	0/4452	0.43	0/6044
1	F	0.27	0/4577	0.44	0/6217
All	All	0.26	0/27266	0.44	0/37033

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

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	56	0
1	B	4542	0	4629	74	0
1	C	4443	0	4529	91	0
1	D	4438	0	4520	79	0
1	E	4376	0	4472	88	0
1	F	4495	0	4580	85	0
2	A	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	435	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 (435) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ARG:NH1	1:F:344:GLU:OE2	2.24	0.70
1:B:439:ILE:HG22	1:B:520:LEU:HB3	1.75	0.69
1:A:37:ARG:NH2	1:D:32:ASN:OD1	2.26	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: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:130:ARG:NH1	1:E:344:GLU:OE2	2.27	0.66
1:E:67:MET:SD	1:E:297:THR:OG1	2.53	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: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:420:ILE:HG13	1:E:425:ILE:HD11	1.81	0.61
1:E:60:TYR:HB2	1:E:303:PHE:HB2	1.82	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:155:LEU:O	1:C:159:LEU:HG	2.05	0.56
1:C:56:LEU:N	1:C:57:PRO:HD2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:150:SER:HB3	1:E:328:GLY:HA2	1.88	0.55
1:E:46:VAL:HG23	1:E:101:ARG:HD3	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: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:F:402:THR:HG23	2:F:701:ANP:O2A	2.07	0.54
1:E:277:ASN:OD1	1:F:91:ARG:HD2	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:291:TRP:NE1	1:E:298:VAL:HG23	2.26	0.51
1:E:64:VAL:HG22	1:E:297:THR:HG21	1.93	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:C:284:MET:HA	1:C:287:THR:HG22	1.93	0.50
1:D:304:VAL:HA	1:D:307:TYR:CZ	2.46	0.50
1:C:284:MET:HB3	1:D:83:PHE:HE2	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:67:MET:HE2	1:C:298:VAL:HG21	1.92	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: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:223:ARG:HD3	1:C:246:ARG:HG2	1.94	0.49
1:C:50:LYS:HE3	1:C:168:GLU:HG3	1.95	0.49
1:E:206:ARG:NH2	1:E:261:SER:O	2.46	0.49
1:B:172:VAL:HG11	1:B:311:LEU:HD22	1.94	0.48
1:B:33:ALA:HB3	1:B:35:LEU:HG	1.95	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
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: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:D:79:VAL:O	1:D:83:PHE:HB3	2.14	0.48
1:E:89:LEU:O	1:E:93:SER:OG	2.22	0.48
2:E:701:ANP:N3B	1:F:499:SER:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:374:ARG:NH1	2:C:701:ANP:O3'	2.40	0.47
1:C:81:LEU:O	1:C:84:VAL:HG12	2.15	0.47
1:E:445:VAL:HG13	1:E:494:ARG:HG2	1.96	0.47
1:B:425:ILE:HG13	1:B:433:LEU:HD13	1.97	0.47
1:B:347:ASP:OD1	1:B:430:GLN:HG3	2.15	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:F:144:ILE:HD13	1:F:335:MET:HE2	1.98	0.46
1:A:146:ARG:NH1	1:A:214:ASN:HB3	2.31	0.46
1:B:276:VAL:HG22	1:B:312:PHE:CD1	2.50	0.46
1:B:78:THR:O	1:B:82:ALA:HB2	2.15	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
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:E:42:ALA:HB1	1:E:101:ARG:HG3	1.97	0.46
1:F:280:MET:HE1	1:F:305:ASN:HA	1.98	0.46
1:F:311:LEU:C	1:F:314:PRO:HD2	2.37	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:476:ILE:HG23	1:C:479:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:PRO:HG3	1:C:307:TYR:OH	2.15	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:F:389:ARG:HG3	1:F:549:THR:HB	1.97	0.44
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: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: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:C:67:MET:HB3	1:C:67:MET:HE2	1.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:408:PHE:CZ	1:D:236:TYR:HA	2.53	0.44
1:B:46:VAL:CG2	1:B:101:ARG:HD3	2.48	0.43
1:A:236:TYR:CD1	1:B:439:ILE:HD11	2.52	0.43
1:D:62:LYS:HZ1	1:D:79:VAL:HA	1.83	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:A:280:MET:HE1	1:A:305:ASN:OD1	2.19	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:HA	1:E:296:LEU:HD23	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:449:ASP:OD1	1:C:450:THR:HG23	2.19	0.43
1:C:85:LEU:HA	1:C:85:LEU:HD23	1.86	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
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:B:52:THR:HG21	1:B:93:SER:OG	2.18	0.43
1:C:336:PHE:O	1:C:339:ILE:HG13	2.18	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: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:F:392:ILE:HB	1:F:552:ILE:HG12	2.00	0.43
1:B:276:VAL:HG13	1:B:312:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:522:ASP:HA	1:E:552:ILE:HB	2.02	0.42
1:E:114:ARG:HG3	1:F:251:ALA:HB1	2.01	0.42
1:F:397:GLY:N	2:F:701:ANP:HNB1	2.11	0.42
1:B:206:ARG:CZ	1:B:323:ARG:HE	2.32	0.42
1:B:26:TYR:O	1:B:29:PRO:HD2	2.20	0.42
1:A:361:VAL:HB	1:A:384:VAL:HB	2.01	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:C:85:LEU:O	1:C:89:LEU:HB2	2.20	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:425:ILE:HG23	1:E:433:LEU:HD22	2.02	0.42
1:E:83:PHE:CE2	1:F:284:MET:HB2	2.54	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:525:THR:OG1	1:C:533:GLU:OE2	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:62:LYS:HD3	1:E:62:LYS:HA	1.81	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:485:GLN:HB2	1:D:489:THR:CG2	2.51	0.41
1:D:62:LYS:CE	1:D:79:VAL:HA	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: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
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:483:LEU:HD13	1:F:489:THR:HG21	2.03	0.41
1:F:454:ASN:O	1:F:510:ARG:HG2	2.21	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: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:D:280:MET:HE3	1:D:305:ASN:HA	2.03	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:363:PHE:CZ	1:A:403:ILE:HG23	2.57	0.40
1:A:291:TRP:HH2	1:B:71:GLY:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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%)	47	78
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%)	47	78
All	All	3440/3684 (93%)	3349 (97%)	89 (3%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	461/491 (94%)	460 (100%)	1 (0%)	93	97
1	B	467/491 (95%)	464 (99%)	3 (1%)	86	93
1	C	456/491 (93%)	455 (100%)	1 (0%)	93	97
1	D	456/491 (93%)	450 (99%)	6 (1%)	69	84
1	E	450/491 (92%)	448 (100%)	2 (0%)	91	95
1	F	462/491 (94%)	461 (100%)	1 (0%)	93	97
All	All	2752/2946 (93%)	2738 (100%)	14 (0%)	88	94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	PHE
1	B	67	MET
1	B	69	LEU
1	B	382	PHE
1	C	312	PHE
1	D	48	LEU
1	D	67	MET
1	D	263	ASN
1	D	307	TYR
1	D	312	PHE
1	D	350	ASN
1	E	52	THR
1	E	312	PHE
1	F	312	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN

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 monosaccharides 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	29,33,33	1.04	4 (13%)	31,52,52	1.19	3 (9%)
2	ANP	B	701	3	29,33,33	1.10	4 (13%)	31,52,52	1.00	3 (9%)
2	ANP	A	701	3	29,33,33	1.08	4 (13%)	31,52,52	1.11	4 (12%)
2	ANP	C	701	3	29,33,33	0.99	2 (6%)	31,52,52	1.14	4 (12%)
2	ANP	E	701	3	29,33,33	1.09	3 (10%)	31,52,52	1.15	3 (9%)
2	ANP	F	701	3	29,33,33	1.10	4 (13%)	31,52,52	1.04	2 (6%)

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	-	3/14/38/38	0/3/3/3
2	ANP	B	701	3	-	4/14/38/38	0/3/3/3
2	ANP	A	701	3	-	1/14/38/38	0/3/3/3
2	ANP	C	701	3	-	5/14/38/38	0/3/3/3
2	ANP	E	701	3	-	6/14/38/38	0/3/3/3
2	ANP	F	701	3	-	3/14/38/38	0/3/3/3

All (21) 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-N3B	2.64	1.70	1.63
2	F	701	ANP	PG-N3B	2.55	1.70	1.63
2	A	701	ANP	PG-O1G	2.55	1.50	1.46
2	B	701	ANP	PG-O1G	2.47	1.50	1.46
2	E	701	ANP	PG-O1G	2.37	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	F	701	ANP	PB-O3A	-2.34	1.56	1.59
2	C	701	ANP	PG-O1G	2.29	1.49	1.46
2	F	701	ANP	PG-O1G	2.29	1.49	1.46
2	F	701	ANP	PB-O1B	2.28	1.49	1.46
2	B	701	ANP	PB-O1B	2.24	1.49	1.46
2	A	701	ANP	PB-O1B	2.23	1.49	1.46
2	D	701	ANP	PG-O1G	2.20	1.49	1.46
2	D	701	ANP	PB-O1B	2.18	1.49	1.46
2	A	701	ANP	PB-N3B	2.11	1.68	1.63
2	B	701	ANP	PB-N3B	2.05	1.68	1.63
2	D	701	ANP	PB-O3A	-2.03	1.56	1.59
2	E	701	ANP	PB-O3A	-2.02	1.56	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	ANP	PA-O3A-PB	-3.54	120.17	132.62
2	A	701	ANP	O3A-PB-N3B	3.43	116.11	106.59
2	E	701	ANP	PA-O3A-PB	-3.32	120.94	132.62
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	B	701	ANP	PA-O3A-PB	-2.74	122.96	132.62
2	C	701	ANP	PA-O3A-PB	-2.71	123.08	132.62
2	E	701	ANP	O1G-PG-N3B	-2.53	108.04	111.77
2	F	701	ANP	C5-C6-N6	2.28	123.82	120.35
2	D	701	ANP	C5-C6-N6	2.27	123.80	120.35
2	C	701	ANP	C5-C6-N6	2.25	123.78	120.35
2	A	701	ANP	C5-C6-N6	2.25	123.78	120.35
2	E	701	ANP	C5-C6-N6	2.25	123.78	120.35
2	A	701	ANP	PA-O3A-PB	-2.24	124.73	132.62
2	C	701	ANP	O1B-PB-N3B	-2.22	108.50	111.77
2	B	701	ANP	C5-C6-N6	2.21	123.71	120.35
2	C	701	ANP	O3A-PB-N3B	2.16	112.58	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 (22) torsion outliers are listed below:

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

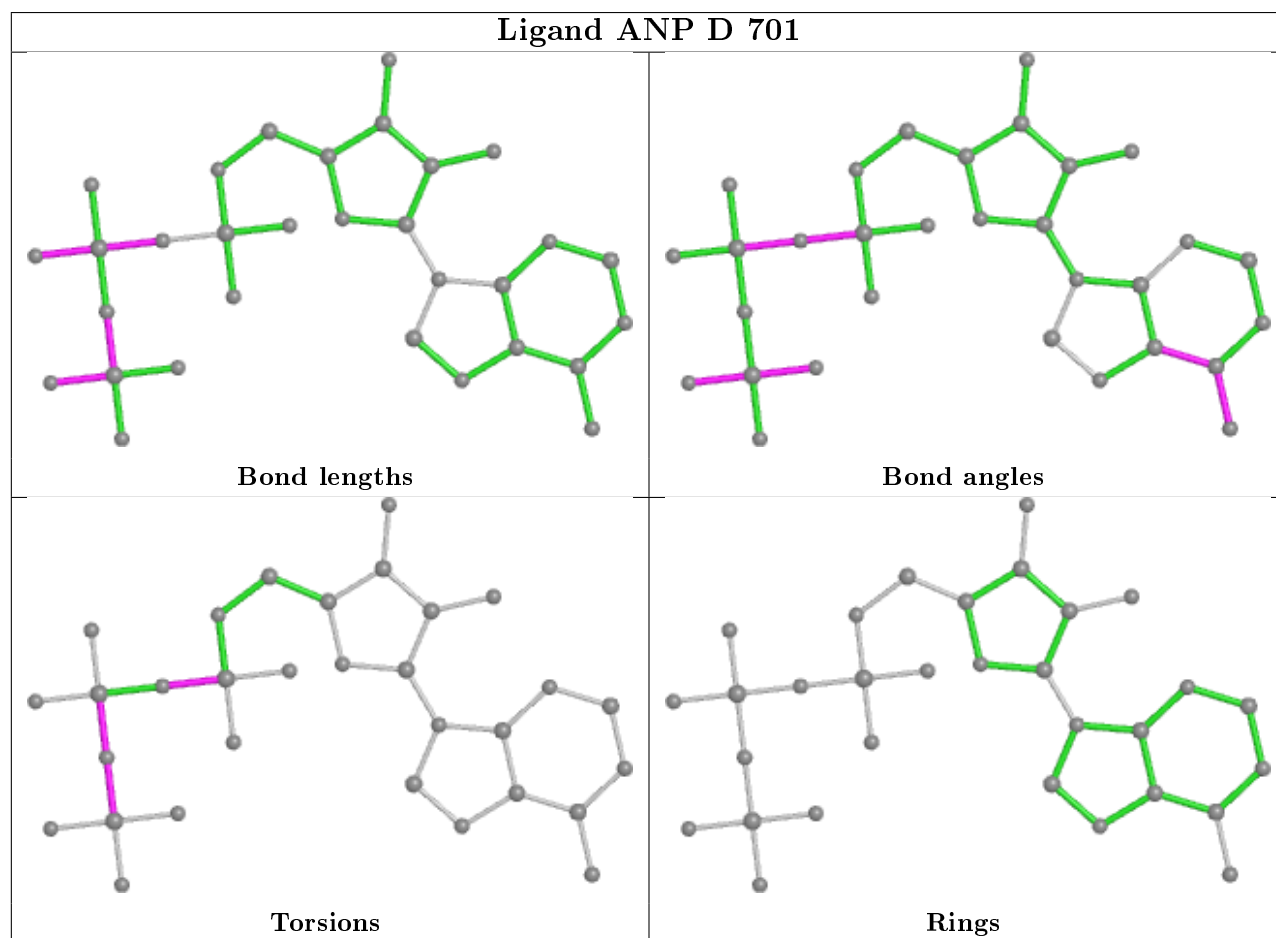
There are no ring outliers.

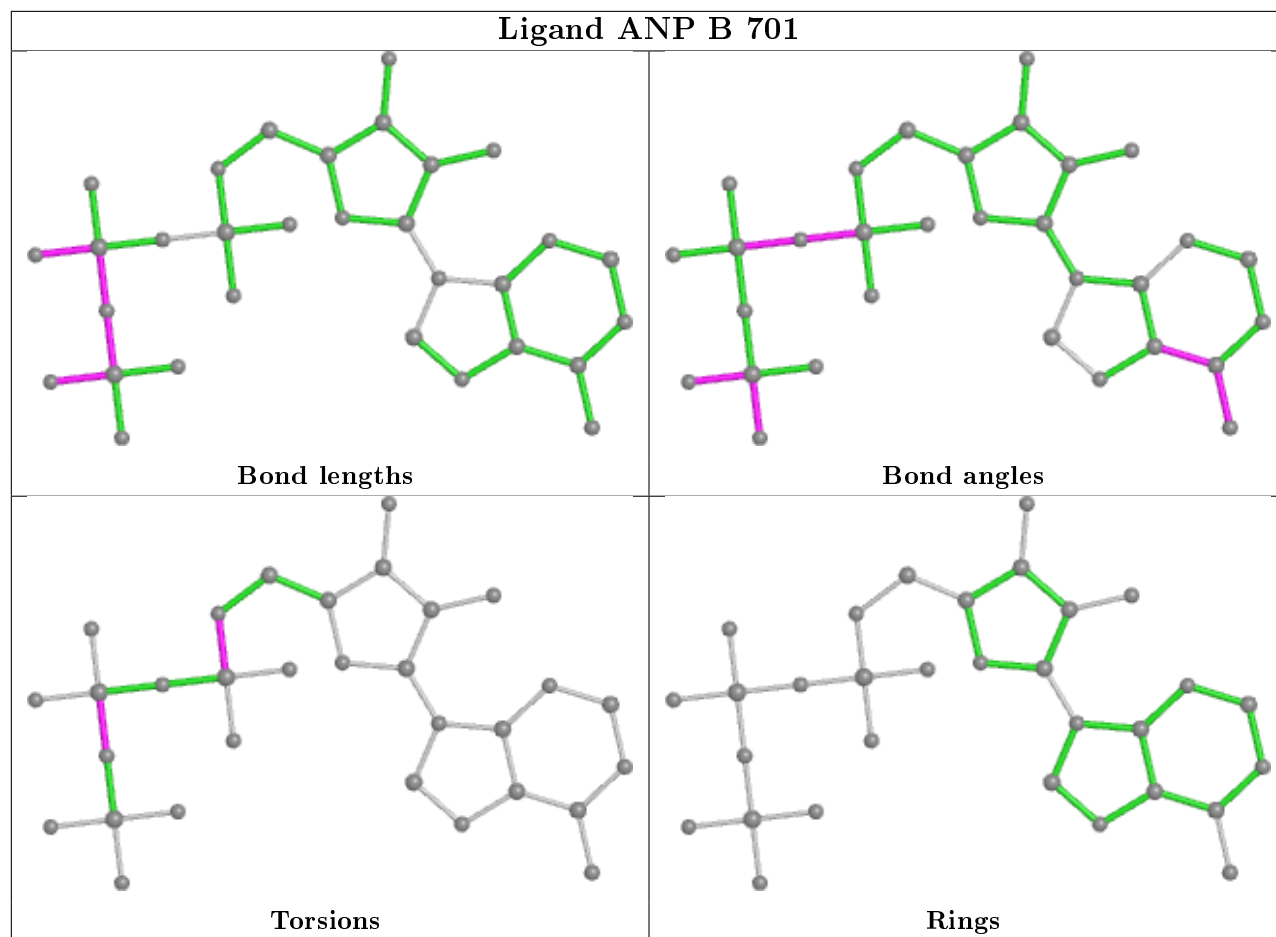
5 monomers are involved in 20 short contacts:

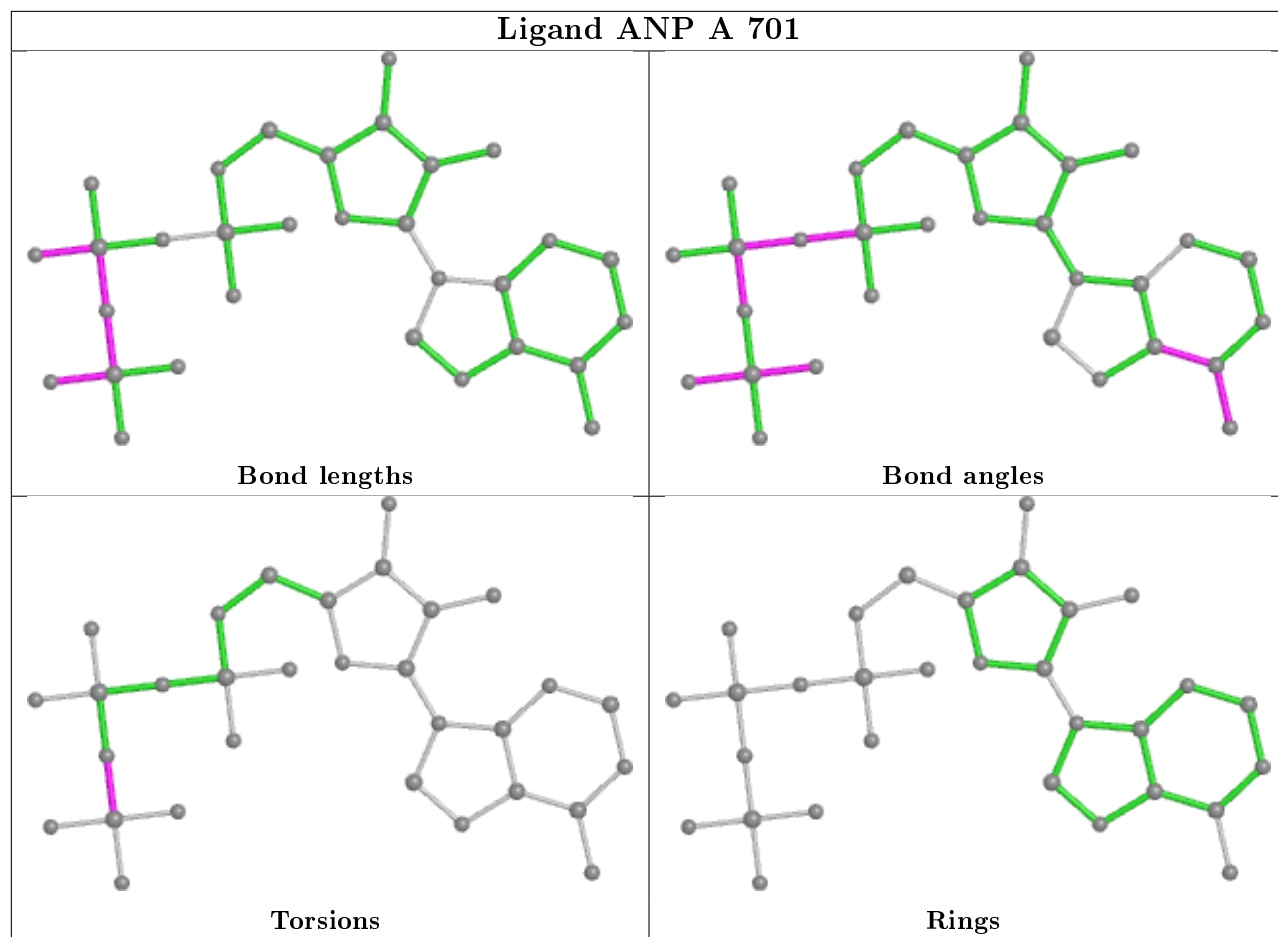
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	ANP	2	0
2	B	701	ANP	1	0
2	C	701	ANP	4	0
2	E	701	ANP	6	0
2	F	701	ANP	7	0

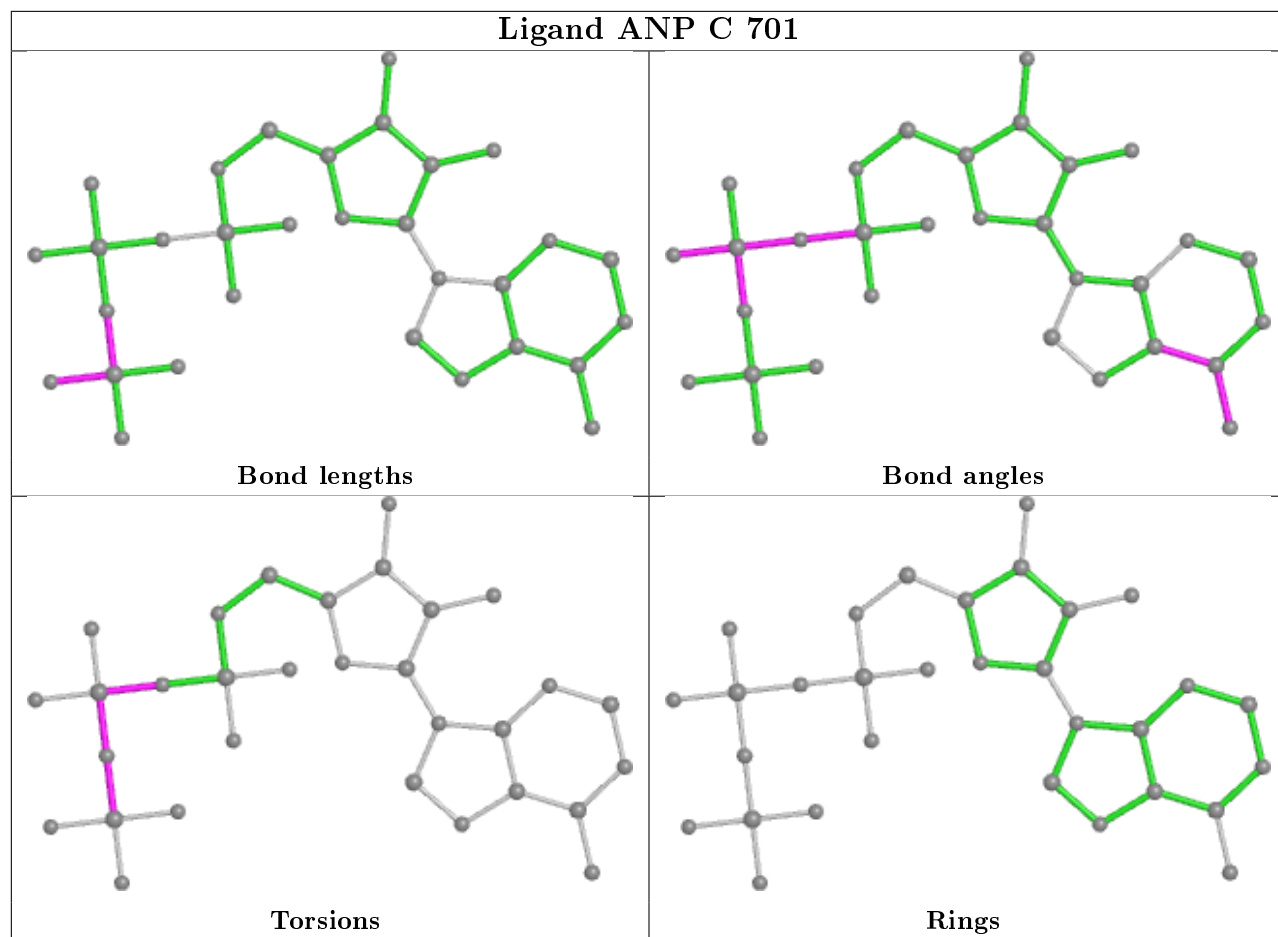
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

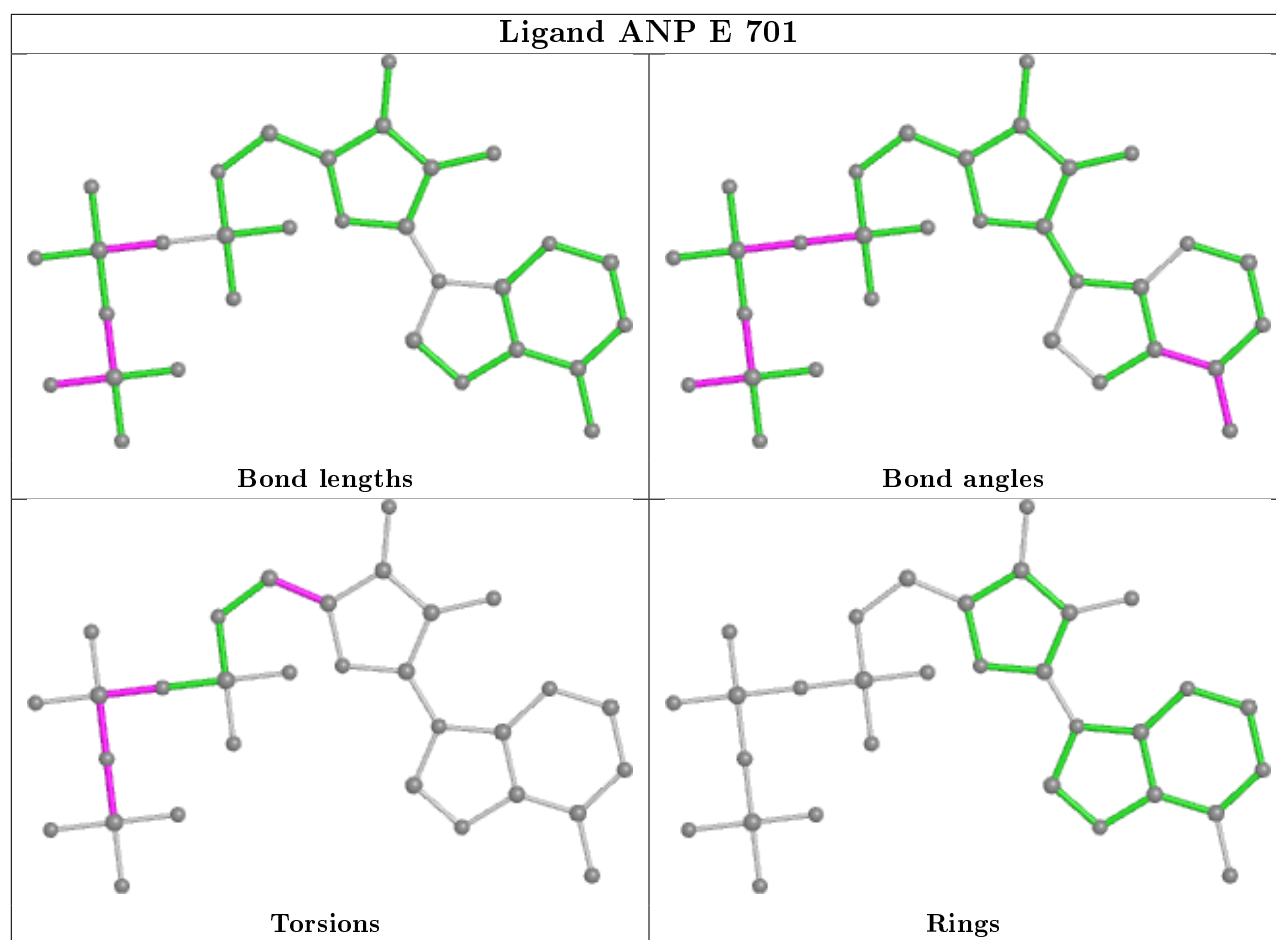
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

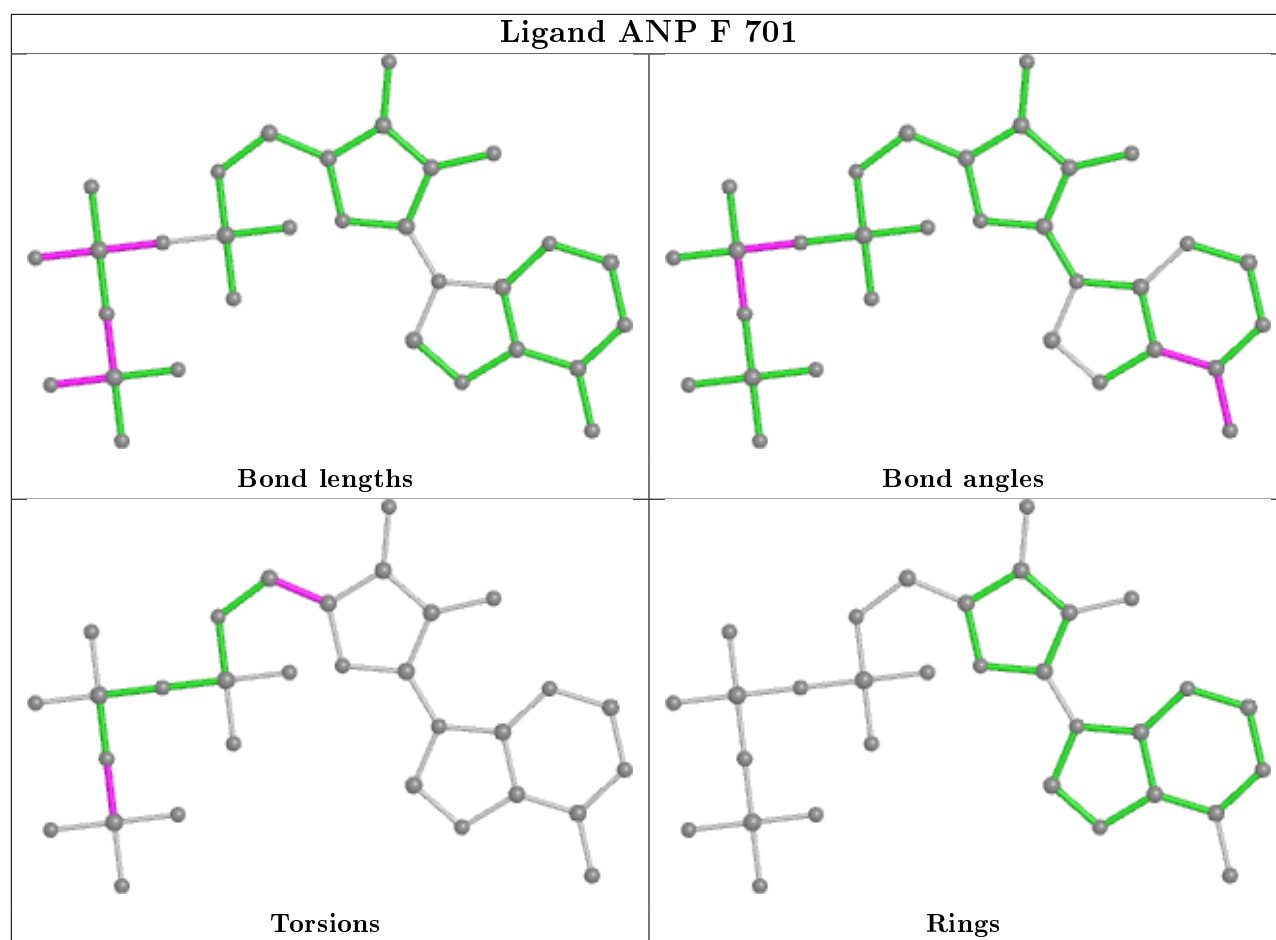












5.7 Other polymers [i](#)

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%)	-0.18	13 (2%) 62 65	27, 64, 123, 187	0
1	B	584/614 (95%)	-0.23	12 (2%) 63 67	34, 66, 118, 181	0
1	C	573/614 (93%)	0.25	46 (8%) 12 14	87, 122, 202, 243	0
1	D	573/614 (93%)	0.23	39 (6%) 17 20	87, 127, 201, 233	0
1	E	565/614 (92%)	0.53	70 (12%) 4 4	58, 120, 304, 330	0
1	F	579/614 (94%)	0.80	101 (17%) 1 1	57, 119, 307, 346	0
All	All	3452/3684 (93%)	0.23	281 (8%) 12 13	27, 106, 262, 346	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	287	THR	14.9
1	F	81	LEU	13.6
1	C	81	LEU	11.7
1	F	67	MET	11.4
1	F	294	GLY	11.0
1	F	68	THR	9.7
1	E	67	MET	9.5
1	F	300	ASP	9.2
1	E	68	THR	8.9
1	F	59	ALA	8.4
1	F	60	TYR	8.2
1	F	600	SER	7.8
1	F	184	LEU	7.7
1	F	282	GLY	7.7
1	C	73	ALA	7.2
1	D	76	ALA	7.1
1	D	295	LYS	7.1
1	F	107	ARG	7.0
1	C	77	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
1	F	299	GLY	6.9
1	C	71	GLY	6.9
1	F	57	PRO	6.9
1	E	271	ALA	6.7
1	E	293	GLN	6.6
1	E	75	PRO	6.4
1	F	286	TRP	6.3
1	C	80	ALA	6.3
1	E	74	GLN	6.2
1	E	208	HIS	6.2
1	E	295	LYS	6.1
1	F	295	LYS	5.9
1	F	296	LEU	5.9
1	E	322	TYR	5.8
1	F	31	ASP	5.8
1	F	306	THR	5.8
1	F	171	ALA	5.7
1	F	58	PHE	5.6
1	F	188	THR	5.6
1	E	69	LEU	5.6
1	E	315	LEU	5.5
1	D	294	GLY	5.4
1	E	77	LEU	5.4
1	F	77	LEU	5.4
1	F	283	ALA	5.4
1	E	76	ALA	5.4
1	D	289	TYR	5.3
1	D	298	VAL	5.3
1	C	72	GLY	5.3
1	F	63	ALA	5.3
1	D	598	ALA	5.3
1	F	30	ALA	5.2
1	E	81	LEU	5.2
1	E	310	GLN	5.2
1	F	186	THR	5.1
1	F	290	GLY	5.1
1	F	292	SER	5.1
1	C	78	THR	5.1
1	F	302	VAL	5.1
1	F	291	TRP	5.0
1	C	67	MET	5.0
1	F	180	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	73	ALA	4.8
1	C	82	ALA	4.8
1	D	70	GLY	4.8
1	F	192	VAL	4.7
1	E	105	PHE	4.6
1	F	176	PHE	4.6
1	F	105	PHE	4.6
1	F	85	LEU	4.6
1	F	190	LEU	4.6
1	F	173	ILE	4.5
1	F	55	ALA	4.5
1	E	267	LEU	4.5
1	F	328	GLY	4.4
1	C	70	GLY	4.4
1	F	297	THR	4.3
1	A	70	GLY	4.3
1	C	295	LYS	4.3
1	D	288	VAL	4.2
1	E	272	GLN	4.2
1	F	54	LEU	4.2
1	C	76	ALA	4.1
1	F	293	GLN	4.1
1	B	85	LEU	4.1
1	F	108	VAL	4.1
1	E	59	ALA	4.1
1	E	309	THR	4.1
1	C	74	GLN	4.0
1	A	599	GLU	4.0
1	B	75	PRO	4.0
1	F	284	MET	4.0
1	F	599	GLU	4.0
1	F	267	LEU	4.0
1	F	80	ALA	4.0
1	F	175	ILE	4.0
1	E	350	ASN	4.0
1	E	289	TYR	3.9
1	F	181	GLY	3.9
1	E	294	GLY	3.9
1	F	289	TYR	3.9
1	F	64	VAL	3.9
1	A	24	LEU	3.9
1	D	75	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	339	ILE	3.9
1	F	109	GLY	3.8
1	E	319	GLY	3.8
1	F	185	VAL	3.8
1	E	195	TYR	3.8
1	D	484	PRO	3.8
1	D	357	ASN	3.7
1	D	337	ARG	3.7
1	C	75	PRO	3.7
1	F	70	GLY	3.7
1	B	252	ARG	3.7
1	C	68	THR	3.7
1	E	311	LEU	3.7
1	E	190	LEU	3.6
1	E	177	TRP	3.6
1	E	186	THR	3.6
1	F	301	LEU	3.6
1	E	182	LEU	3.5
1	A	27	LEU	3.5
1	E	259	VAL	3.5
1	D	74	GLN	3.5
1	E	291	TRP	3.5
1	F	168	GLU	3.5
1	E	282	GLY	3.5
1	E	102	ASN	3.4
1	C	443	ASP	3.4
1	F	288	VAL	3.4
1	E	78	THR	3.4
1	E	80	ALA	3.4
1	F	78	THR	3.4
1	F	56	LEU	3.4
1	E	85	LEU	3.3
1	B	81	LEU	3.3
1	E	312	PHE	3.3
1	E	64	VAL	3.3
1	E	349	PRO	3.3
1	D	65	ASP	3.2
1	D	71	GLY	3.2
1	F	342	HIS	3.2
1	C	35	LEU	3.2
1	E	308	LEU	3.2
1	E	290	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	310	GLN	3.2
1	A	23	PHE	3.2
1	E	73	ALA	3.2
1	D	338	LEU	3.2
1	C	374	ARG	3.2
1	E	70	GLY	3.1
1	B	72	GLY	3.1
1	C	209	LEU	3.1
1	C	463	SER	3.1
1	E	60	TYR	3.1
1	F	303	PHE	3.1
1	C	462	ALA	3.1
1	E	268	LEU	3.1
1	A	25	PRO	3.0
1	D	31	ASP	3.0
1	C	442	GLN	3.0
1	F	71	GLY	3.0
1	C	85	LEU	3.0
1	C	37	ARG	3.0
1	E	98	ASP	3.0
1	E	209	LEU	3.0
1	D	252	ARG	3.0
1	F	69	LEU	2.9
1	D	597	ALA	2.9
1	E	314	PRO	2.9
1	C	289	TYR	2.9
1	F	584	ARG	2.9
1	D	178	LEU	2.9
1	E	278	LEU	2.9
1	D	317	MET	2.8
1	F	258	ALA	2.8
1	E	292	SER	2.8
1	B	65	ASP	2.8
1	F	349	PRO	2.8
1	D	293	GLN	2.8
1	F	32	ASN	2.8
1	C	34	VAL	2.8
1	C	334	GLU	2.8
1	D	442	GLN	2.8
1	D	443	ASP	2.8
1	C	267	LEU	2.7
1	C	27	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	30	ALA	2.7
1	E	79	VAL	2.7
1	F	304	VAL	2.7
1	E	444	SER	2.7
1	C	444	SER	2.7
1	F	330	ILE	2.7
1	C	373	ASP	2.7
1	E	274	LEU	2.6
1	D	362	THR	2.6
1	E	58	PHE	2.6
1	F	357	ASN	2.6
1	F	179	ASN	2.6
1	E	100	LEU	2.6
1	E	353	ALA	2.6
1	C	178	LEU	2.6
1	C	338	LEU	2.6
1	F	263	ASN	2.6
1	C	487	TYR	2.6
1	F	82	ALA	2.6
1	C	350	ASN	2.6
1	F	37	ARG	2.6
1	E	260	LYS	2.6
1	E	298	VAL	2.5
1	D	327	GLN	2.5
1	F	183	GLY	2.5
1	D	481	ALA	2.5
1	D	599	GLU	2.5
1	B	543	VAL	2.5
1	D	80	ALA	2.5
1	D	285	ALA	2.5
1	F	61	LYS	2.5
1	E	156	TYR	2.5
1	F	172	VAL	2.5
1	A	350	ASN	2.4
1	D	182	LEU	2.4
1	F	174	VAL	2.4
1	F	193	ILE	2.4
1	F	298	VAL	2.4
1	F	598	ALA	2.4
1	B	77	LEU	2.4
1	A	29	PRO	2.4
1	D	333	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	293	GLN	2.4
1	D	350	ASN	2.4
1	F	443	ASP	2.4
1	F	583	LEU	2.4
1	C	256	ASP	2.4
1	C	330	ILE	2.4
1	F	84	VAL	2.3
1	C	543	VAL	2.3
1	E	264	SER	2.3
1	C	208	HIS	2.3
1	F	324	THR	2.3
1	D	104	VAL	2.3
1	E	313	ARG	2.3
1	D	482	ARG	2.3
1	E	71	GLY	2.3
1	F	260	LYS	2.3
1	A	32	ASN	2.2
1	F	338	LEU	2.2
1	F	152	ASP	2.2
1	F	160	PHE	2.2
1	F	335	MET	2.2
1	E	56	LEU	2.2
1	F	23	PHE	2.2
1	F	75	PRO	2.2
1	E	299	GLY	2.2
1	F	27	LEU	2.2
1	D	596	GLN	2.2
1	D	593	TRP	2.1
1	D	290	GLY	2.1
1	C	40	VAL	2.1
1	F	38	ARG	2.1
1	A	598	ALA	2.1
1	F	34	VAL	2.1
1	B	76	ALA	2.1
1	C	296	LEU	2.1
1	E	443	ASP	2.1
1	B	260	LYS	2.1
1	E	154	MET	2.1
1	C	283	ALA	2.1
1	A	73	ALA	2.1
1	F	595	ARG	2.1
1	E	580	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	178	LEU	2.1
1	B	182	LEU	2.0
1	D	68	THR	2.0
1	E	199	THR	2.0
1	F	189	ILE	2.0
1	C	337	ARG	2.0
1	E	37	ARG	2.0
1	C	306	THR	2.0
1	C	65	ASP	2.0
1	A	181	GLY	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](#)

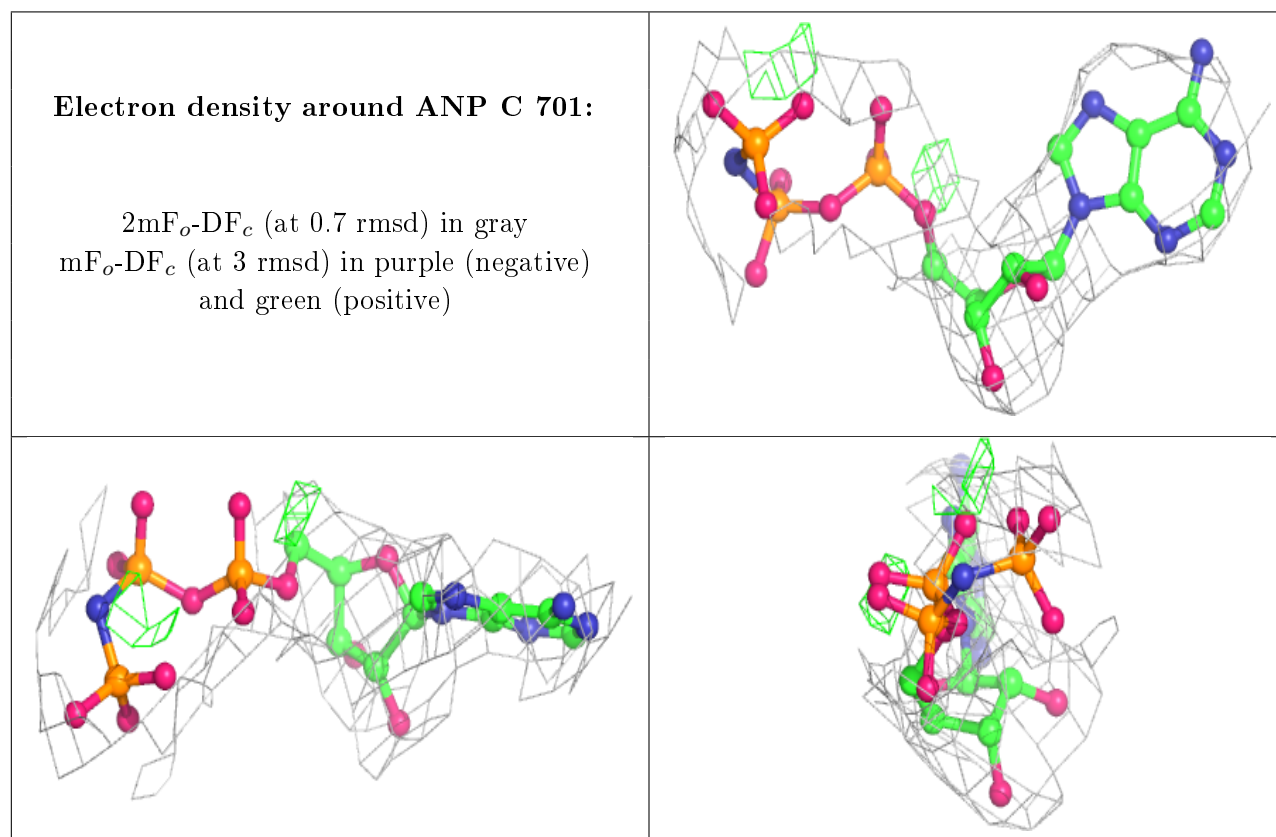
There are no monosaccharides in this entry.

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.

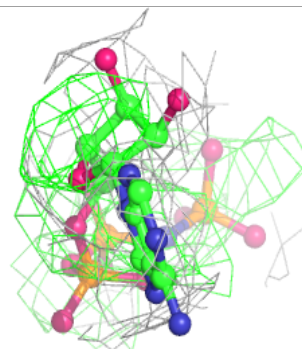
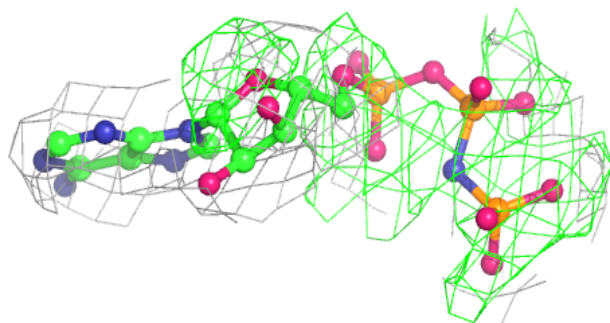
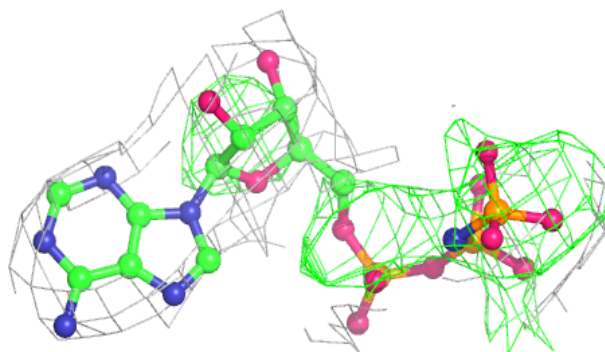
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	F	702	1/1	0.86	0.33	64,64,64,64	0
3	MG	B	702	1/1	0.89	0.44	49,49,49,49	0
2	ANP	C	701	31/31	0.91	0.29	103,139,160,178	0
2	ANP	E	701	31/31	0.91	0.31	86,117,141,153	0
2	ANP	F	701	31/31	0.91	0.31	74,98,125,129	0
3	MG	C	702	1/1	0.92	0.44	116,116,116,116	0
3	MG	A	702	1/1	0.93	0.41	36,36,36,36	0
2	ANP	D	701	31/31	0.93	0.28	102,124,134,138	0
2	ANP	A	701	31/31	0.94	0.27	38,58,83,99	0
2	ANP	B	701	31/31	0.95	0.34	40,71,82,96	0
3	MG	E	702	1/1	0.96	0.30	52,52,52,52	0
3	MG	D	702	1/1	0.96	0.41	87,87,87,87	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.

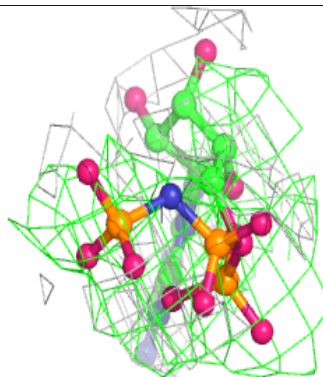
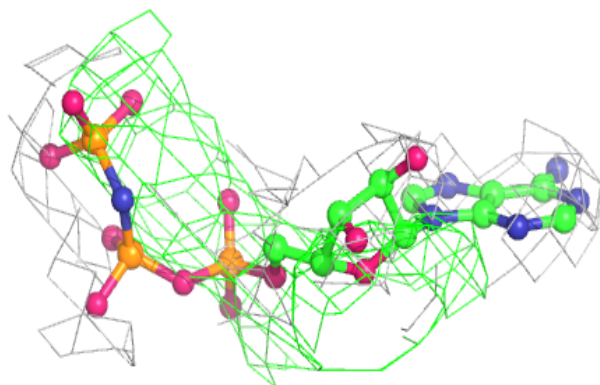
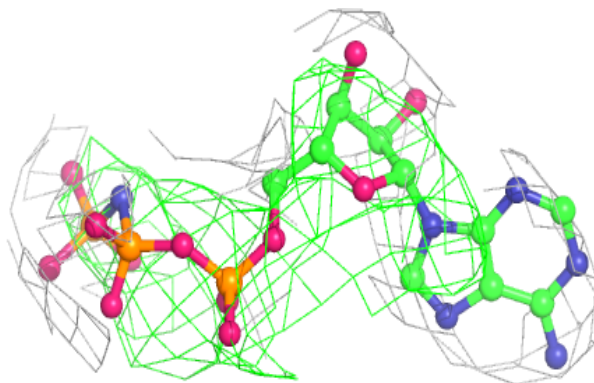


Electron density around ANP E 701:

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

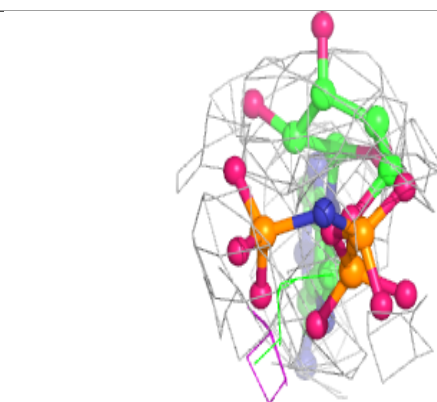
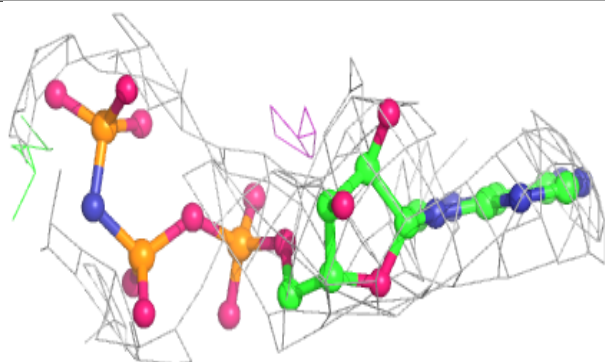
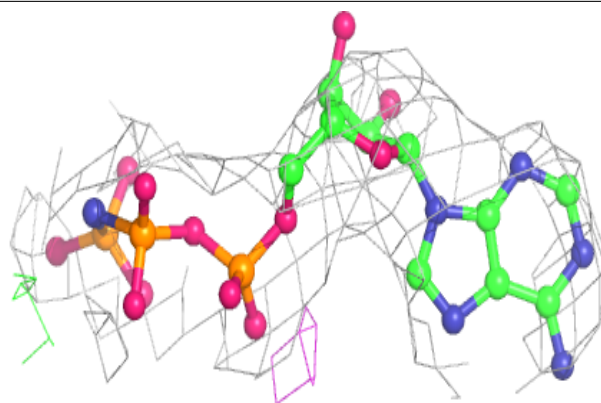
**Electron density around ANP F 701:**

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

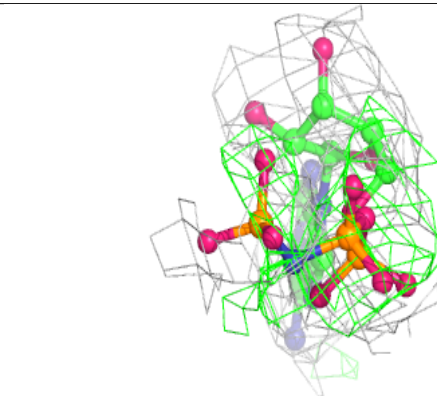
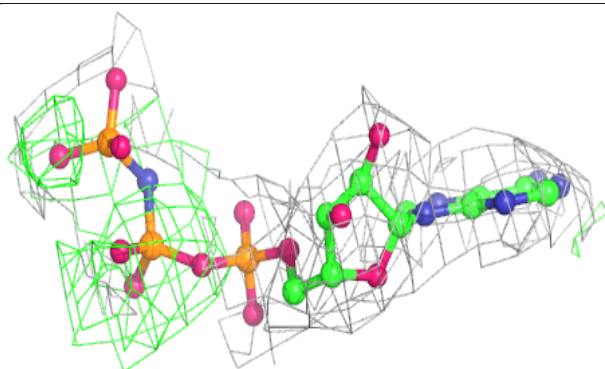
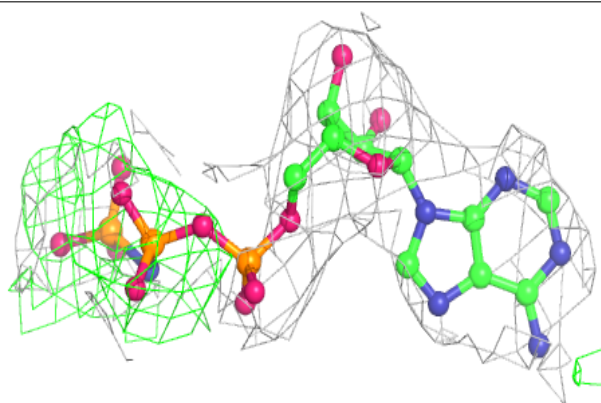


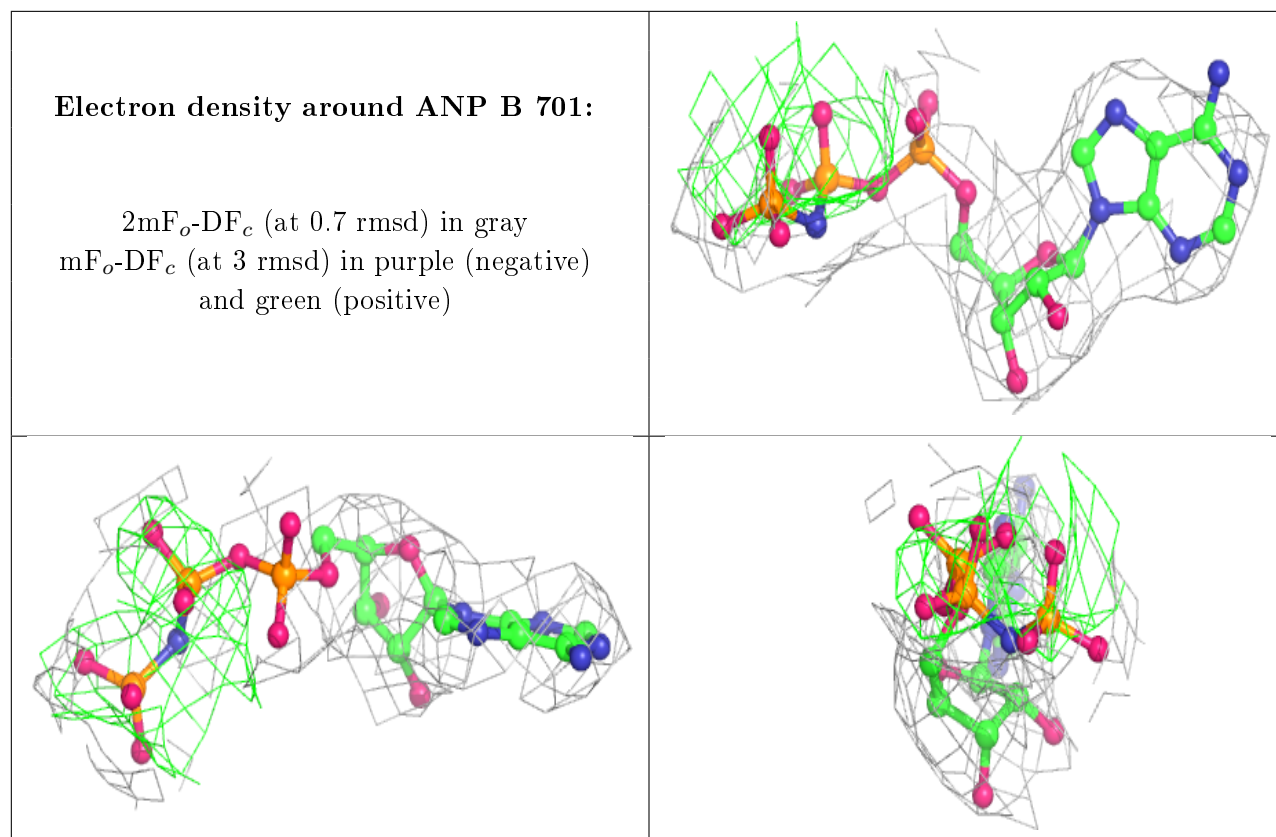
Electron density around ANP D 701:

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

**Electron density around ANP 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.