Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 09:34 PM JST

PDB ID	:	7WUA
Title	:	Crystal structures of FadD32 from Corynebacterium diphtheriae
Authors	:	Liu, X.
Deposited on	:	2022-02-07
Resolution	:	2.00 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:

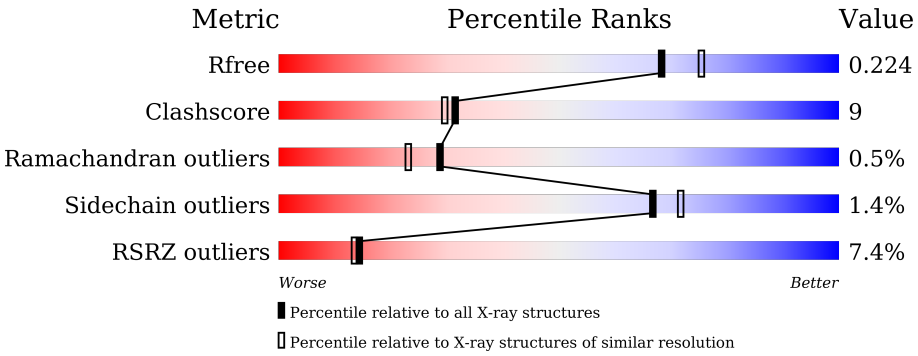
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	604	4% 87% 12%
1	B	604	9% 80% 19%
1	C	604	11% 79% 17%
1	D	604	4% 69% 12% 19%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19768 atoms, of which 160 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.

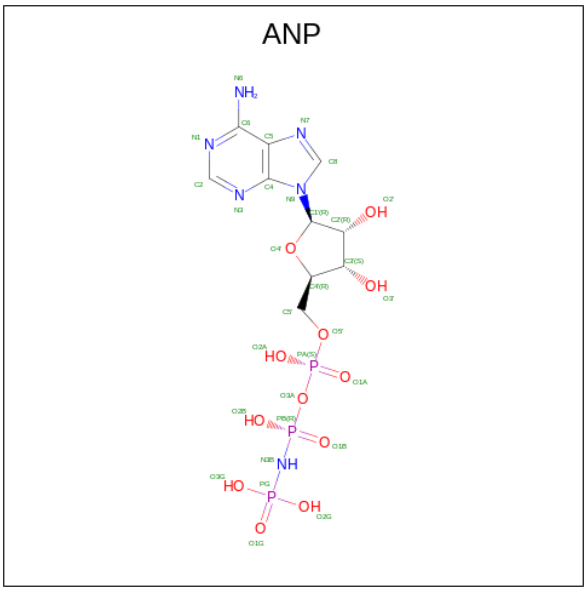
- Molecule 1 is a protein called Acyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4618	2910	813	884	11			
1	B	597	Total	C	N	O	S	0	0	0
			4578	2887	805	875	11			
1	C	593	Total	C	N	O	S	0	0	0
			4531	2860	795	865	11			
1	D	490	Total	C	N	O	S	0	0	0
			3758	2381	652	714	11			

There are 4 discrepancies between the modelled and reference sequences:

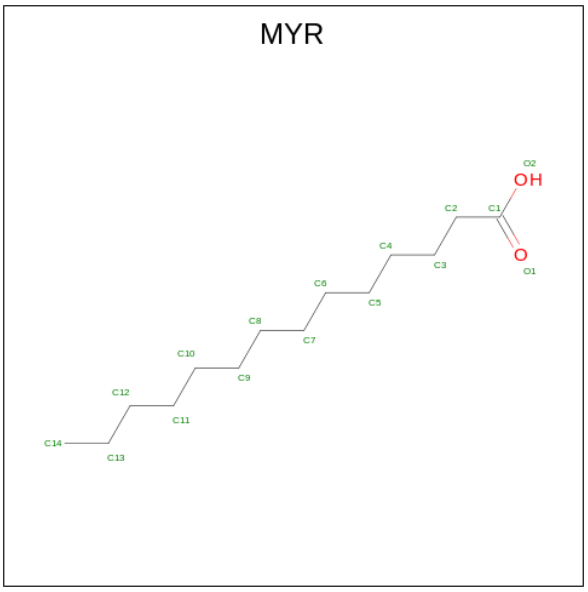
Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ILE	VAL	conflict	UNP A0A679LZK7
B	254	ILE	VAL	conflict	UNP A0A679LZK7
C	254	ILE	VAL	conflict	UNP A0A679LZK7
D	254	ILE	VAL	conflict	UNP A0A679LZK7

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	C	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	D	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		

- Molecule 3 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 43 14 27 2	0	0
3	B	1	Total C H O 43 14 27 2	0	0
3	C	1	Total C H O 43 14 27 2	0	0
3	D	1	Total C H O 43 14 27 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

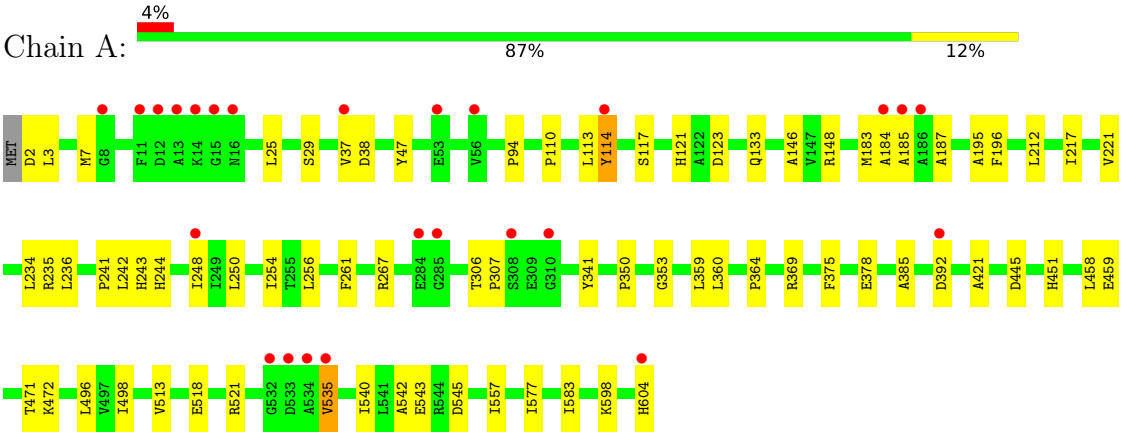
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	589	Total O 589 589	0	0
5	B	421	Total O 421 421	0	0
5	C	482	Total O 482 482	0	0
5	D	441	Total O 441 441	0	0

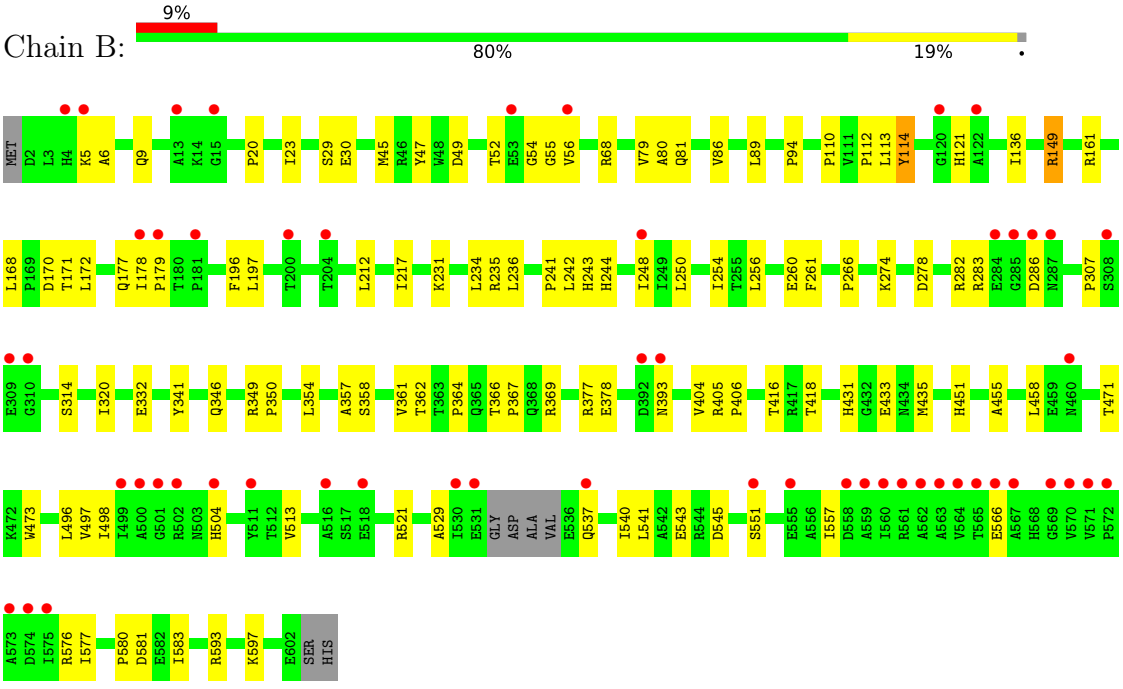
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Acyl-CoA synthase

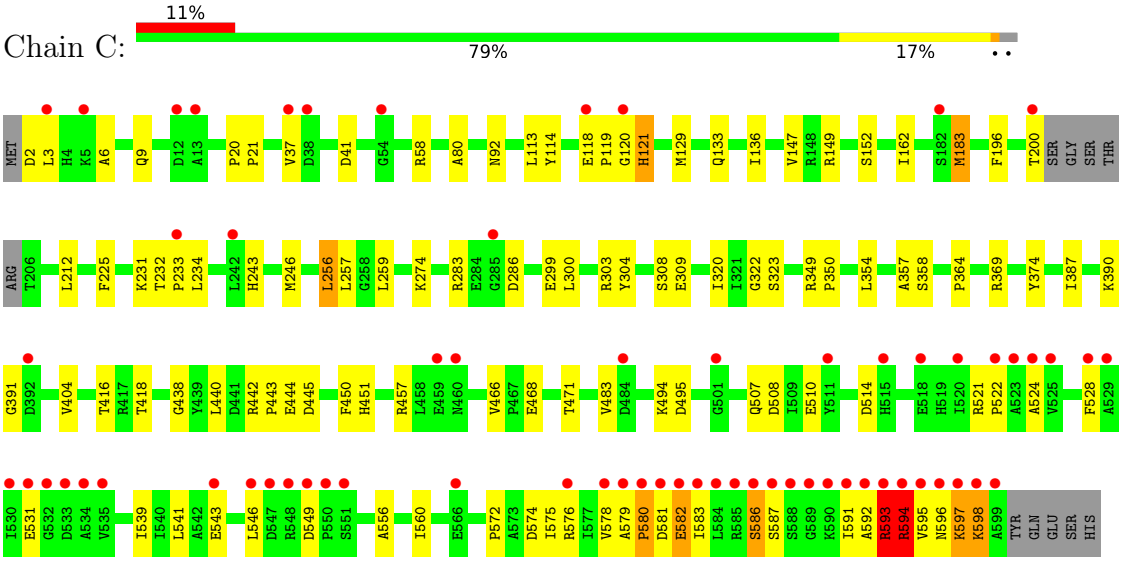


• Molecule 1: Acyl-CoA synthase



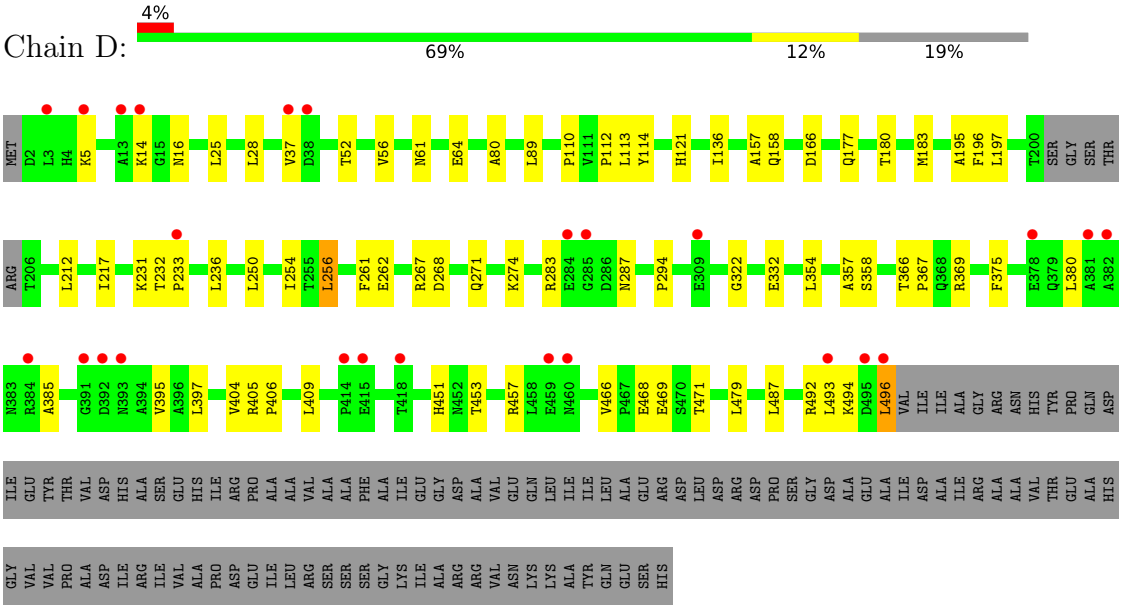
• Molecule 1: Acyl-CoA synthase

Chain C:



• Molecule 1: Acyl-CoA synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.65Å 97.53Å 142.04Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	46.10 – 2.00 47.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (46.10-2.00) 97.2 (47.26-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.185 , 0.224 0.187 , 0.224	Depositor DCC
R_{free} test set	9564 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19768	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, MYR, 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	0.36	0/4715	0.53	0/6432
1	B	0.30	0/4673	0.48	0/6373
1	C	0.38	0/4625	0.58	2/6311 (0.0%)
1	D	0.33	0/3840	0.51	1/5241 (0.0%)
All	All	0.34	0/17853	0.52	3/24357 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	586	SER	C-N-CA	5.65	135.82	121.70
1	D	256	LEU	CA-CB-CG	5.04	126.88	115.30
1	C	593	ARG	N-CA-CB	5.02	119.64	110.60

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	4618	0	4566	57	0
1	B	4578	0	4532	86	0
1	C	4531	0	4482	108	0
1	D	3758	0	3718	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	13	12	1	0
2	B	31	13	12	1	0
2	C	31	13	12	3	0
2	D	31	13	12	1	0
3	A	16	27	27	1	0
3	B	16	27	27	1	0
3	C	16	27	27	5	0
3	D	16	27	27	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	589	0	0	20	0
5	B	421	0	0	15	0
5	C	482	0	0	17	0
5	D	441	0	0	14	0
All	All	19608	160	17454	316	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 9.

All (316) 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:C:583:ILE:CG2	1:C:595:VAL:HG21	1.59	1.31
2:B:701:ANP:O4'	2:B:701:ANP:C1'	1.65	1.23
2:A:701:ANP:O4'	2:A:701:ANP:C1'	1.65	1.16
1:C:583:ILE:HG21	1:C:595:VAL:HG21	1.12	1.09
1:C:129:MET:SD	5:C:1208:HOH:O	2.15	1.03
1:C:583:ILE:HD13	1:C:595:VAL:HG11	1.38	1.02
1:D:479:LEU:CD1	1:D:496:LEU:HD11	1.92	0.98
1:D:479:LEU:HD11	1:D:496:LEU:HD11	1.45	0.98
1:C:583:ILE:HG21	1:C:595:VAL:CG2	1.93	0.98
1:B:212:LEU:HD13	1:B:217:ILE:HD11	1.44	0.98
1:A:535:VAL:CG2	5:A:1102:HOH:O	2.15	0.94
1:C:579:ALA:O	1:C:581:ASP:N	2.02	0.93
1:A:535:VAL:HG23	5:A:1102:HOH:O	1.72	0.87
1:D:479:LEU:HD21	1:D:493:LEU:HD13	1.58	0.86
1:B:231:LYS:NZ	5:B:801:HOH:O	2.08	0.85
1:D:177:GLN:NE2	5:D:802:HOH:O	2.09	0.85
1:C:528:PHE:CD2	1:C:594:ARG:HD2	2.11	0.84
1:C:583:ILE:CG2	1:C:595:VAL:CG2	2.52	0.78
1:D:492:ARG:NH2	1:D:494:LYS:HE2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:ILE:HD13	1:C:574:ASP:HB3	1.64	0.78
1:B:177:GLN:NE2	5:B:807:HOH:O	2.18	0.76
1:B:496:LEU:HD23	1:B:498:ILE:HD11	1.66	0.76
1:A:378:GLU:OE2	5:A:801:HOH:O	2.02	0.76
1:A:25:LEU:HD22	1:A:256:LEU:HD21	1.67	0.75
1:A:148:ARG:HD2	5:A:809:HOH:O	1.86	0.75
1:D:492:ARG:CZ	1:D:494:LYS:HE2	2.16	0.75
1:C:256:LEU:HD23	1:C:257:LEU:CD1	2.17	0.75
1:C:92:ASN:ND2	5:C:803:HOH:O	2.16	0.74
1:C:443:PRO:HD2	5:C:812:HOH:O	1.87	0.74
1:A:212:LEU:HD13	1:A:217:ILE:HD11	1.70	0.73
1:B:149:ARG:NH2	5:B:809:HOH:O	2.21	0.73
1:C:539:ILE:HD12	1:C:597:LYS:NZ	2.05	0.72
1:C:583:ILE:HG22	1:C:595:VAL:HG21	1.69	0.72
1:D:37:VAL:O	5:D:801:HOH:O	2.08	0.72
1:A:378:GLU:OE1	5:A:802:HOH:O	2.06	0.72
1:A:518:GLU:OE1	5:A:803:HOH:O	2.08	0.71
1:D:52:THR:HB	1:D:56:VAL:HG23	1.73	0.70
1:B:81:GLN:OE1	5:B:802:HOH:O	2.09	0.70
1:C:387:ILE:HD11	1:C:483:VAL:HG11	1.72	0.70
1:C:521:ARG:NH1	1:C:580:PRO:HB3	2.07	0.70
1:D:158:GLN:HG3	5:D:995:HOH:O	1.91	0.70
1:B:196:PHE:CZ	1:B:212:LEU:HD12	2.27	0.69
1:B:541:LEU:HD13	1:B:576:ARG:HB3	1.73	0.69
1:C:543:GLU:OE2	1:C:582:GLU:HB2	1.92	0.69
1:C:541:LEU:HD23	1:C:576:ARG:HB3	1.75	0.69
1:C:256:LEU:HD23	1:C:257:LEU:HD12	1.75	0.69
1:A:236:LEU:HD21	1:A:250:LEU:HG	1.74	0.69
1:B:551:SER:O	5:B:803:HOH:O	2.11	0.68
1:B:282:ARG:NH2	1:B:314:SER:OG	2.23	0.68
1:B:171:THR:OG1	5:B:804:HOH:O	2.12	0.67
1:C:583:ILE:HD13	1:C:595:VAL:CG1	2.19	0.67
1:B:20:PRO:HG2	1:B:23:ILE:CG1	2.24	0.67
1:B:20:PRO:HG2	1:B:23:ILE:HG12	1.77	0.67
1:C:583:ILE:CB	1:C:595:VAL:HG21	2.24	0.67
1:D:453:THR:OG1	1:D:471:THR:HG22	1.95	0.67
1:A:37:VAL:O	5:A:805:HOH:O	2.13	0.66
1:C:528:PHE:CG	1:C:594:ARG:HD2	2.30	0.66
1:C:6:ALA:O	1:C:9:GLN:HG2	1.96	0.66
1:A:445:ASP:OD2	5:A:807:HOH:O	2.14	0.66
1:A:267:ARG:NH2	5:A:808:HOH:O	2.18	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:GLU:CD	1:C:580:PRO:HA	2.16	0.65
1:D:271:GLN:HG2	5:D:1062:HOH:O	1.96	0.65
1:D:25:LEU:HD11	1:D:217:ILE:HG21	1.78	0.65
1:C:80:ALA:HB2	1:C:136:ILE:HD11	1.78	0.65
2:C:701:ANP:O1B	5:C:802:HOH:O	2.14	0.65
1:D:232:THR:O	5:D:804:HOH:O	2.14	0.65
1:A:235:ARG:HD2	5:A:847:HOH:O	1.97	0.64
1:B:557:ILE:HG13	1:B:577:ILE:HD12	1.79	0.64
1:D:287:ASN:O	5:D:805:HOH:O	2.15	0.64
1:D:114:TYR:CE1	1:D:121:HIS:HB3	2.33	0.64
1:C:514:ASP:OD1	1:C:522:PRO:HA	1.97	0.64
1:D:180:THR:HG23	5:D:935:HOH:O	1.97	0.64
1:C:3:LEU:HD21	1:C:259:LEU:HD11	1.81	0.63
1:C:524:ALA:HA	1:C:591:ILE:HD11	1.81	0.63
1:B:458:LEU:O	5:B:805:HOH:O	2.16	0.63
1:A:360:LEU:HD13	3:A:702:MYR:H72	1.80	0.63
1:C:80:ALA:HB2	1:C:136:ILE:CD1	2.29	0.62
1:C:457:ARG:NH2	1:C:466:VAL:O	2.23	0.62
1:D:267:ARG:HD3	5:D:813:HOH:O	2.00	0.62
1:C:37:VAL:HG12	5:C:811:HOH:O	2.00	0.61
1:A:25:LEU:HD11	1:A:217:ILE:HG21	1.83	0.61
1:B:283:ARG:HB3	5:B:894:HOH:O	2.01	0.61
1:A:29:SER:HB2	1:A:256:LEU:HG	1.84	0.60
1:C:303:ARG:HD2	1:C:304:TYR:CE2	2.37	0.60
1:C:118:GLU:HG2	1:C:119:PRO:HD2	1.82	0.60
1:B:433:GLU:OE1	5:B:806:HOH:O	2.16	0.60
1:C:539:ILE:HD12	1:C:597:LYS:HZ2	1.67	0.60
1:C:543:GLU:OE2	1:C:582:GLU:N	2.27	0.60
1:B:178:ILE:H	1:B:178:ILE:HD12	1.65	0.59
1:B:161:ARG:NH2	5:B:811:HOH:O	2.22	0.59
1:C:308:SER:HB3	5:C:877:HOH:O	2.01	0.59
1:B:29:SER:HB2	1:B:256:LEU:HD12	1.84	0.58
1:C:442:ARG:HA	5:C:809:HOH:O	2.03	0.58
1:B:114:TYR:CE1	1:B:121:HIS:HB3	2.39	0.58
1:B:377:ARG:HB3	1:B:393:ASN:ND2	2.18	0.58
1:A:148:ARG:NH1	5:A:809:HOH:O	2.19	0.58
1:B:52:THR:HG22	1:B:54:GLY:N	2.18	0.58
1:A:2:ASP:N	5:A:819:HOH:O	2.37	0.58
1:B:566:GLU:OE1	1:B:566:GLU:HA	2.03	0.58
1:D:479:LEU:HD12	1:D:496:LEU:HD11	1.79	0.57
1:B:283:ARG:O	1:B:286:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:CD2	1:A:250:LEU:HG	2.35	0.57
1:D:268:ASP:OD2	5:D:807:HOH:O	2.18	0.57
1:C:539:ILE:CD1	1:C:574:ASP:HB3	2.33	0.57
1:D:395:VAL:HG23	1:D:397:LEU:HD13	1.86	0.57
1:C:3:LEU:HD23	1:C:225:PHE:HE2	1.69	0.56
1:C:444:GLU:HG2	1:C:445:ASP:N	2.20	0.56
1:B:593:ARG:NH2	5:B:825:HOH:O	2.39	0.56
1:D:80:ALA:HB2	1:D:136:ILE:CD1	2.35	0.56
1:D:80:ALA:HB2	1:D:136:ILE:HD11	1.85	0.56
1:C:41:ASP:HB2	5:C:822:HOH:O	2.04	0.56
1:B:178:ILE:HD12	1:B:178:ILE:N	2.21	0.56
1:B:307:PRO:HG2	1:B:341:TYR:CE1	2.41	0.56
1:D:492:ARG:NH1	1:D:494:LYS:HE2	2.20	0.55
1:C:120:GLY:O	1:C:121:HIS:ND1	2.40	0.55
1:C:521:ARG:HH12	1:C:580:PRO:HB3	1.71	0.55
1:D:496:LEU:O	1:D:496:LEU:HD22	2.08	0.54
1:D:233:PRO:HA	5:D:856:HOH:O	2.08	0.54
1:C:583:ILE:HG21	1:C:595:VAL:HG11	1.90	0.54
1:D:457:ARG:NH2	1:D:466:VAL:O	2.29	0.54
1:B:236:LEU:HD21	1:B:250:LEU:HG	1.88	0.54
1:A:236:LEU:HD21	1:A:250:LEU:CG	2.37	0.54
1:C:531:GLU:O	1:C:531:GLU:HG3	2.07	0.54
1:A:451:HIS:HA	1:A:471:THR:O	2.07	0.54
1:A:196:PHE:CZ	1:A:212:LEU:HD12	2.44	0.53
1:C:594:ARG:HG2	1:C:598:LYS:HZ1	1.74	0.53
1:A:123:ASP:HB2	5:A:850:HOH:O	2.09	0.53
1:B:361:VAL:HG12	1:B:362:THR:HG23	1.91	0.53
1:A:472:LYS:NZ	5:A:814:HOH:O	2.30	0.52
1:C:583:ILE:HD12	1:C:595:VAL:HB	1.90	0.52
1:D:16:ASN:HB2	5:D:806:HOH:O	2.09	0.52
1:D:110:PRO:HD2	1:D:195:ALA:O	2.09	0.52
1:C:539:ILE:HD12	1:C:597:LYS:HZ1	1.73	0.52
1:B:451:HIS:HA	1:B:471:THR:O	2.09	0.52
1:C:283:ARG:O	1:C:286:ASP:HB2	2.10	0.52
1:A:543:GLU:HG3	1:A:583:ILE:HD12	1.92	0.52
1:B:497:VAL:HB	1:B:504:HIS:O	2.09	0.52
1:A:236:LEU:HD21	1:A:250:LEU:CD2	2.40	0.52
1:D:157:ALA:HB3	5:D:995:HOH:O	2.09	0.52
1:A:234:LEU:HD12	1:A:234:LEU:C	2.31	0.52
1:D:357:ALA:O	1:D:358:SER:HB2	2.09	0.52
1:A:521:ARG:HB2	1:A:545:ASP:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ALA:HB2	1:B:136:ILE:HD11	1.92	0.51
1:B:254:ILE:HG21	1:B:261:PHE:HB2	1.91	0.51
1:C:468:GLU:HG3	5:C:1009:HOH:O	2.10	0.51
1:D:89:LEU:HD23	1:D:113:LEU:HB2	1.93	0.51
1:C:303:ARG:HD2	1:C:304:TYR:CZ	2.46	0.51
1:D:262:GLU:CD	1:D:283:ARG:HH22	2.13	0.50
1:D:405:ARG:HB3	1:D:406:PRO:HA	1.94	0.50
1:B:529:ALA:HA	1:B:537:GLN:O	2.12	0.50
1:B:377:ARG:HB3	1:B:393:ASN:HD21	1.76	0.49
1:C:391:GLY:O	5:C:804:HOH:O	2.19	0.49
1:A:392:ASP:HB2	5:A:834:HOH:O	2.10	0.49
1:A:38:ASP:O	5:A:810:HOH:O	2.19	0.49
1:A:242:LEU:O	1:A:248:ILE:HB	2.12	0.49
1:A:254:ILE:HG21	1:A:261:PHE:CD1	2.46	0.49
1:C:594:ARG:HE	1:C:598:LYS:NZ	2.10	0.49
1:D:5:LYS:HG2	5:D:1086:HOH:O	2.12	0.49
1:C:440:LEU:O	1:C:442:ARG:HG3	2.12	0.49
1:C:357:ALA:O	1:C:358:SER:HB2	2.13	0.49
1:D:451:HIS:HA	1:D:471:THR:O	2.12	0.49
1:B:89:LEU:HD23	1:B:113:LEU:HB2	1.95	0.49
1:C:543:GLU:HA	1:C:578:VAL:O	2.12	0.49
1:A:25:LEU:HD22	1:A:256:LEU:CD2	2.39	0.49
1:B:250:LEU:HD11	3:B:702:MYR:H112	1.94	0.48
1:C:507:GLN:HA	1:C:510:GLU:OE1	2.12	0.48
1:C:541:LEU:CD2	1:C:576:ARG:HB3	2.41	0.48
1:C:576:ARG:HD3	5:C:1081:HOH:O	2.14	0.48
1:D:375:PHE:CD2	1:D:397:LEU:HD22	2.48	0.48
1:A:496:LEU:HD23	1:A:498:ILE:HD11	1.96	0.48
1:C:200:THR:HA	5:C:1017:HOH:O	2.13	0.48
1:A:114:TYR:CE1	1:A:121:HIS:HB3	2.48	0.48
1:A:513:VAL:HG21	1:A:540:ILE:HD13	1.96	0.48
1:B:47:TYR:CG	1:B:94:PRO:HD3	2.48	0.48
1:B:274:LYS:HE3	1:B:278:ASP:OD1	2.14	0.48
1:C:113:LEU:O	1:C:243:HIS:HB3	2.14	0.48
5:A:979:HOH:O	1:D:183:MET:HG3	2.13	0.48
1:B:52:THR:HG22	1:B:55:GLY:H	1.79	0.48
1:B:332:GLU:HA	1:B:332:GLU:OE1	2.13	0.48
1:A:113:LEU:O	1:A:243:HIS:HB3	2.14	0.47
1:C:583:ILE:CD1	1:C:595:VAL:HG11	2.27	0.47
1:B:112:PRO:HD2	1:B:197:LEU:O	2.14	0.47
1:C:457:ARG:HG3	5:C:997:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:GLU:N	1:D:469:GLU:OE1	2.47	0.47
1:D:236:LEU:HD21	1:D:250:LEU:HD21	1.97	0.47
1:D:404:VAL:O	1:D:404:VAL:HG23	2.15	0.47
1:B:6:ALA:O	1:B:9:GLN:HG2	2.14	0.46
1:B:242:LEU:O	1:B:248:ILE:HB	2.15	0.46
1:D:14:LYS:HE2	1:D:14:LYS:HB3	1.53	0.46
1:A:557:ILE:HG13	1:A:577:ILE:HD12	1.97	0.46
1:D:375:PHE:CE1	1:D:385:ALA:HB1	2.51	0.46
1:C:451:HIS:HA	1:C:471:THR:O	2.16	0.46
1:D:468:GLU:OE1	5:D:808:HOH:O	2.21	0.46
1:C:149:ARG:O	1:C:152:SER:OG	2.24	0.46
1:B:404:VAL:O	1:B:404:VAL:HG23	2.16	0.46
1:C:320:ILE:HG13	3:C:702:MYR:H122	1.98	0.46
1:B:45:MET:HA	1:B:261:PHE:O	2.15	0.46
1:D:28:LEU:HD23	1:D:256:LEU:HD11	1.97	0.46
1:D:114:TYR:HE1	1:D:121:HIS:HB3	1.80	0.46
1:A:133:GLN:NE2	5:A:824:HOH:O	2.39	0.46
1:C:231:LYS:HB3	1:C:231:LYS:HE3	1.70	0.46
1:B:235:ARG:HB3	1:B:260:GLU:HB3	1.98	0.45
5:B:1011:HOH:O	1:C:183:MET:HE1	2.16	0.45
1:A:375:PHE:CE1	1:A:385:ALA:HB1	2.52	0.45
1:B:29:SER:CA	1:B:256:LEU:HD12	2.47	0.45
1:C:309:GLU:O	5:C:805:HOH:O	2.21	0.45
1:C:596:ASN:HA	1:C:598:LYS:HE2	1.97	0.45
1:B:521:ARG:HB2	1:B:545:ASP:HA	1.99	0.45
1:D:496:LEU:C	1:D:496:LEU:CD2	2.85	0.45
1:A:2:ASP:N	5:A:838:HOH:O	2.49	0.45
1:B:236:LEU:CD2	1:B:250:LEU:HG	2.46	0.45
1:B:346:GLN:HG2	1:B:346:GLN:O	2.16	0.45
2:C:701:ANP:PA	3:C:702:MYR:O2	2.75	0.45
1:D:166:ASP:OD1	1:D:166:ASP:N	2.49	0.45
1:B:29:SER:HA	1:B:256:LEU:HD12	1.99	0.45
1:B:52:THR:HG22	1:B:54:GLY:H	1.81	0.45
1:C:495:ASP:OD2	1:C:593:ARG:NH2	2.47	0.45
1:C:507:GLN:HG2	1:C:508:ASP:N	2.32	0.45
1:B:29:SER:CB	1:B:256:LEU:HD12	2.47	0.45
1:A:110:PRO:HD2	1:A:195:ALA:O	2.18	0.44
1:C:354:LEU:HD23	1:C:354:LEU:N	2.31	0.44
1:C:594:ARG:HE	1:C:598:LYS:HZ1	1.65	0.44
1:D:492:ARG:HH22	1:D:494:LYS:HE2	1.79	0.44
1:B:30:GLU:OE1	1:B:30:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TYR:CG	1:A:94:PRO:HD3	2.53	0.44
1:C:438:GLY:HA2	1:C:450:PHE:CE2	2.53	0.44
1:D:409:LEU:HD21	1:D:487:LEU:HD22	1.99	0.44
1:A:254:ILE:HG21	1:A:261:PHE:HB2	1.99	0.44
1:B:378:GLU:HG2	5:B:839:HOH:O	2.18	0.44
2:C:701:ANP:O1A	3:C:702:MYR:O2	2.36	0.44
1:C:232:THR:HA	1:C:233:PRO:C	2.38	0.44
1:C:416:THR:O	1:C:418:THR:HG23	2.17	0.44
1:D:375:PHE:CE2	1:D:397:LEU:HB2	2.53	0.44
1:D:254:ILE:HG21	1:D:261:PHE:CD1	2.53	0.44
1:A:513:VAL:CG2	1:A:540:ILE:HD13	2.48	0.44
1:B:49:ASP:OD2	5:B:810:HOH:O	2.21	0.44
1:B:241:PRO:HD3	1:B:266:PRO:HG3	1.99	0.44
1:B:241:PRO:HG2	1:B:244:HIS:CG	2.52	0.43
1:C:583:ILE:HG21	1:C:595:VAL:CG1	2.48	0.43
1:C:598:LYS:HZ3	1:C:598:LYS:HG3	1.75	0.43
1:B:366:THR:HB	1:B:367:PRO:HD2	2.00	0.43
2:D:701:ANP:O2A	3:D:702:MYR:O1	2.36	0.43
1:A:234:LEU:HD11	1:A:254:ILE:HD11	1.99	0.43
1:B:357:ALA:O	1:B:358:SER:HB2	2.18	0.43
1:B:593:ARG:HG3	1:B:593:ARG:NH1	2.33	0.43
1:B:235:ARG:HA	1:B:260:GLU:O	2.17	0.43
1:C:322:GLY:O	1:C:323:SER:CB	2.67	0.43
1:D:112:PRO:HD2	1:D:197:LEU:O	2.19	0.43
1:B:350:PRO:O	1:B:364:PRO:HD3	2.18	0.43
1:B:416:THR:O	1:B:418:THR:HG23	2.18	0.43
1:D:380:LEU:CD2	1:D:395:VAL:HG21	2.49	0.43
1:A:350:PRO:O	1:A:364:PRO:HD3	2.19	0.43
1:A:421:ALA:HA	1:A:458:LEU:HD11	1.99	0.43
1:C:246:MET:SD	3:C:702:MYR:H62	2.59	0.43
1:C:300:LEU:HD12	1:C:300:LEU:HA	1.90	0.43
1:C:598:LYS:HG3	1:C:598:LYS:H	1.53	0.43
1:D:479:LEU:HD12	1:D:496:LEU:CD1	2.47	0.43
1:B:236:LEU:HD21	1:B:250:LEU:CD2	2.49	0.42
1:A:306:THR:HA	5:A:870:HOH:O	2.19	0.42
1:B:529:ALA:O	1:B:597:LYS:NZ	2.31	0.42
1:B:580:PRO:O	1:B:581:ASP:HB2	2.19	0.42
1:D:366:THR:HB	1:D:367:PRO:HD2	2.01	0.42
1:C:20:PRO:HA	1:C:21:PRO:HD3	1.95	0.42
1:C:323:SER:HA	3:C:702:MYR:O1	2.20	0.42
1:C:404:VAL:HG23	1:C:404:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:ILE:CD1	1:C:595:VAL:CG1	2.93	0.42
1:C:444:GLU:CD	1:C:444:GLU:H	2.22	0.42
1:A:3:LEU:HD23	1:A:3:LEU:HA	1.89	0.42
1:B:543:GLU:HG2	1:B:583:ILE:HG13	2.01	0.42
1:A:7:MET:HE1	1:A:221:VAL:HG12	2.02	0.42
1:C:374:TYR:CE2	1:C:390:LYS:HB2	2.55	0.42
1:B:405:ARG:HB3	1:B:406:PRO:HA	2.01	0.42
1:B:541:LEU:CD1	1:B:576:ARG:HB3	2.46	0.42
1:C:438:GLY:HA2	1:C:450:PHE:CD2	2.54	0.42
1:C:147:VAL:HG12	1:C:162:ILE:HD13	2.02	0.41
1:D:332:GLU:HA	1:D:332:GLU:OE1	2.20	0.41
1:A:542:ALA:O	1:A:577:ILE:HA	2.20	0.41
1:B:56:VAL:HA	5:B:903:HOH:O	2.20	0.41
1:B:354:LEU:N	1:B:354:LEU:HD23	2.34	0.41
1:C:114:TYR:CE1	1:C:121:HIS:HB3	2.56	0.41
1:C:556:ALA:O	1:C:560:ILE:HG13	2.20	0.41
1:B:113:LEU:O	1:B:243:HIS:HB3	2.20	0.41
1:D:196:PHE:CZ	1:D:212:LEU:HD12	2.55	0.41
1:C:543:GLU:OE2	1:C:581:ASP:N	2.54	0.41
1:B:234:LEU:C	1:B:234:LEU:HD12	2.40	0.41
1:B:168:LEU:HB3	1:B:172:LEU:HD12	2.02	0.41
1:D:354:LEU:N	1:D:354:LEU:HD23	2.35	0.41
1:C:320:ILE:HD13	1:C:349:ARG:HB2	2.02	0.41
1:C:350:PRO:O	1:C:364:PRO:HD3	2.20	0.41
1:B:68:ARG:NH1	1:B:170:ASP:OD1	2.54	0.41
1:B:178:ILE:HG23	1:B:179:PRO:HD2	2.02	0.41
1:C:303:ARG:NH1	1:C:304:TYR:OH	2.53	0.41
1:C:444:GLU:CG	1:C:445:ASP:N	2.84	0.41
1:D:61:ASN:OD1	1:D:64:GLU:HG3	2.21	0.41
1:C:543:GLU:HG2	1:C:579:ALA:O	2.21	0.41
1:A:241:PRO:HG2	1:A:244:HIS:ND1	2.36	0.40
1:B:79:VAL:HG23	1:B:136:ILE:CD1	2.51	0.40
1:B:455:ALA:HA	1:C:133:GLN:OE1	2.21	0.40
1:C:546:LEU:CD2	1:C:580:PRO:HG2	2.50	0.40
1:B:513:VAL:HG21	1:B:540:ILE:HD13	2.04	0.40
1:C:234:LEU:C	1:C:234:LEU:HD12	2.42	0.40
1:C:299:GLU:HB2	5:C:848:HOH:O	2.20	0.40
1:C:543:GLU:OE1	1:C:580:PRO:HA	2.21	0.40
1:D:294:PRO:HA	1:D:322:GLY:O	2.21	0.40
1:A:307:PRO:HG2	1:A:341:TYR:CE1	2.56	0.40
1:B:431:HIS:HB2	1:B:473:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ARG:HD2	5:C:1184:HOH:O	2.20	0.40
1:C:196:PHE:CZ	1:C:212:LEU:HD12	2.57	0.40
1:A:117:SER:HB3	1:A:146:ALA:CB	2.51	0.40
1:A:375:PHE:CD1	1:A:385:ALA:HB1	2.56	0.40
1:B:86:VAL:O	1:B:110:PRO:HA	2.21	0.40
1:B:320:ILE:HD13	1:B:349:ARG:HB2	2.03	0.40
1:A:353:GLY:HA3	1:A:359:LEU:O	2.21	0.40
1:B:557:ILE:HG13	1:B:577:ILE:CD1	2.49	0.40
1:C:2:ASP:N	5:C:841:HOH:O	2.53	0.40
1:C:572:PRO:HG2	1:C:575:ILE:HD11	2.03	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	601/604 (100%)	583 (97%)	14 (2%)	4 (1%)	22 16
1	B	593/604 (98%)	577 (97%)	16 (3%)	0	100 100
1	C	589/604 (98%)	557 (95%)	25 (4%)	7 (1%)	13 7
1	D	486/604 (80%)	473 (97%)	13 (3%)	0	100 100
All	All	2269/2416 (94%)	2190 (96%)	68 (3%)	11 (0%)	29 23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ALA
1	A	187	ALA
1	C	587	SER
1	C	593	ARG
1	C	594	ARG

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Mol	Chain	Res	Type
1	A	185	ALA
1	C	580	PRO
1	C	597	LYS
1	C	592	ALA
1	C	121	HIS
1	A	535	VAL

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	482/483 (100%)	476 (99%)	6 (1%)	71	76
1	B	478/483 (99%)	473 (99%)	5 (1%)	76	81
1	C	471/483 (98%)	461 (98%)	10 (2%)	53	57
1	D	394/483 (82%)	390 (99%)	4 (1%)	76	81
All	All	1825/1932 (94%)	1800 (99%)	25 (1%)	67	72

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	TYR
1	A	183	MET
1	A	369	ARG
1	A	459	GLU
1	A	598	LYS
1	A	604	HIS
1	B	5	LYS
1	B	114	TYR
1	B	149	ARG
1	B	369	ARG
1	B	435	MET
1	C	183	MET
1	C	256	LEU
1	C	274	LYS
1	C	369	ARG

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Mol	Chain	Res	Type
1	C	494	LYS
1	C	549	ASP
1	C	582	GLU
1	C	586	SER
1	C	594	ARG
1	C	598	LYS
1	D	231	LYS
1	D	274	LYS
1	D	369	ARG
1	D	496	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN
1	B	393	ASN
1	B	460	ASN
1	C	460	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MYR	A	702	-	15,15,15	0.62	0	15,15,15	0.76	0
2	ANP	A	701	4	29,33,33	4.76	14 (48%)	31,52,52	2.05	6 (19%)
2	ANP	D	701	-	29,33,33	4.64	16 (55%)	31,52,52	3.17	10 (32%)
3	MYR	B	702	-	15,15,15	0.59	0	15,15,15	0.75	0
2	ANP	B	701	4	29,33,33	5.60	18 (62%)	31,52,52	2.86	12 (38%)
3	MYR	C	702	-	15,15,15	0.59	0	15,15,15	0.68	0
3	MYR	D	702	-	15,15,15	0.59	0	15,15,15	0.77	0
2	ANP	C	701	-	29,33,33	5.13	20 (68%)	31,52,52	2.87	11 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MYR	A	702	-	-	7/13/13/13	-
2	ANP	A	701	4	-	6/14/38/38	0/3/3/3
2	ANP	D	701	-	-	6/14/38/38	0/3/3/3
3	MYR	B	702	-	-	6/13/13/13	-
2	ANP	B	701	4	-	7/14/38/38	0/3/3/3
3	MYR	C	702	-	-	9/13/13/13	-
3	MYR	D	702	-	-	7/13/13/13	-
2	ANP	C	701	-	-	7/14/38/38	0/3/3/3

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ANP	O4'-C1'	17.74	1.65	1.41
2	B	701	ANP	O4'-C1'	17.42	1.65	1.41
2	D	701	ANP	O4'-C1'	15.46	1.62	1.41
2	C	701	ANP	O4'-C1'	14.99	1.62	1.41
2	C	701	ANP	C2'-C1'	-11.34	1.36	1.53
2	D	701	ANP	C2'-C1'	-11.01	1.37	1.53
2	A	701	ANP	C2'-C1'	-10.93	1.37	1.53
2	B	701	ANP	C2'-C1'	-10.23	1.38	1.53
2	B	701	ANP	PB-O1B	-9.84	1.30	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ANP	O4'-C4'	-9.44	1.23	1.45
2	D	701	ANP	O4'-C4'	-8.37	1.26	1.45
2	C	701	ANP	O4'-C4'	-8.21	1.26	1.45
2	C	701	ANP	PB-O3A	8.06	1.69	1.59
2	B	701	ANP	PG-O3G	-7.53	1.36	1.56
2	D	701	ANP	O3'-C3'	-7.22	1.26	1.43
2	B	701	ANP	PG-O1G	-7.13	1.34	1.46
2	B	701	ANP	O3'-C3'	-6.99	1.26	1.43
2	C	701	ANP	O3'-C3'	-6.96	1.26	1.43
2	C	701	ANP	PG-N3B	6.44	1.80	1.63
2	D	701	ANP	PB-O2B	-6.09	1.40	1.56
2	A	701	ANP	O4'-C4'	-6.07	1.31	1.45
2	A	701	ANP	PB-O3A	5.76	1.66	1.59
2	A	701	ANP	PG-N3B	5.70	1.78	1.63
2	B	701	ANP	PB-O2B	-5.48	1.42	1.56
2	B	701	ANP	PG-O2G	-5.38	1.42	1.56
2	C	701	ANP	PG-O1G	-5.27	1.37	1.46
2	A	701	ANP	O3'-C3'	-5.17	1.30	1.43
2	C	701	ANP	PB-O2B	-4.95	1.43	1.56
2	B	701	ANP	PG-N3B	4.55	1.75	1.63
2	A	701	ANP	C3'-C4'	4.33	1.64	1.53
2	C	701	ANP	PG-O3G	-4.02	1.45	1.56
2	C	701	ANP	PG-O2G	-3.99	1.46	1.56
2	B	701	ANP	PA-O2A	-3.97	1.36	1.55
2	D	701	ANP	PA-O2A	-3.76	1.37	1.55
2	C	701	ANP	C3'-C4'	3.69	1.62	1.53
2	D	701	ANP	C3'-C4'	3.65	1.62	1.53
2	C	701	ANP	C8-N7	-3.57	1.28	1.34
2	C	701	ANP	PA-O2A	-3.56	1.38	1.55
2	A	701	ANP	O2'-C2'	3.40	1.51	1.43
2	A	701	ANP	PG-O3G	-3.39	1.47	1.56
2	C	701	ANP	C2-N3	-3.35	1.26	1.32
2	B	701	ANP	C3'-C4'	3.32	1.61	1.53
2	B	701	ANP	C8-N7	-3.27	1.28	1.34
2	A	701	ANP	PB-N3B	3.24	1.71	1.63
2	A	701	ANP	PB-O2B	-3.22	1.48	1.56
2	D	701	ANP	C8-N7	-3.16	1.29	1.34
2	D	701	ANP	PG-N3B	3.08	1.71	1.63
2	C	701	ANP	PB-O1B	-2.98	1.41	1.46
2	D	701	ANP	PG-O2G	-2.92	1.48	1.56
2	C	701	ANP	PB-N3B	2.86	1.70	1.63
2	A	701	ANP	PB-O1B	2.82	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	ANP	PB-O3A	2.65	1.62	1.59
2	D	701	ANP	PG-O1G	-2.63	1.42	1.46
2	D	701	ANP	C2-N3	-2.60	1.27	1.32
2	C	701	ANP	C5-N7	-2.55	1.30	1.39
2	B	701	ANP	C5-C4	-2.55	1.34	1.40
2	B	701	ANP	C5-N7	-2.53	1.30	1.39
2	D	701	ANP	PG-O3G	-2.49	1.50	1.56
2	B	701	ANP	PA-O1A	-2.47	1.42	1.50
2	A	701	ANP	PG-O2G	-2.47	1.50	1.56
2	C	701	ANP	PA-O1A	-2.43	1.42	1.50
2	C	701	ANP	C4-N3	-2.41	1.32	1.35
2	A	701	ANP	C6-N6	2.30	1.42	1.34
2	B	701	ANP	PB-N3B	2.29	1.69	1.63
2	B	701	ANP	C2-N3	-2.29	1.28	1.32
2	D	701	ANP	C5-N7	-2.26	1.31	1.39
2	D	701	ANP	C5-C4	-2.13	1.35	1.40
2	C	701	ANP	C6-N6	2.01	1.41	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	ANP	O1B-PB-N3B	-13.03	92.58	111.77
2	C	701	ANP	O1B-PB-N3B	-9.97	97.10	111.77
2	B	701	ANP	O2B-PB-O1B	-8.63	91.83	109.92
2	B	701	ANP	O3G-PG-O1G	-6.93	96.03	113.45
2	A	701	ANP	C3'-C2'-C1'	6.60	110.92	100.98
2	B	701	ANP	N3-C2-N1	-6.37	118.72	128.68
2	D	701	ANP	N3-C2-N1	-5.87	119.50	128.68
2	C	701	ANP	N3-C2-N1	-5.57	119.97	128.68
2	D	701	ANP	O3A-PB-N3B	5.32	121.35	106.59
2	B	701	ANP	C4-C5-N7	-5.24	103.94	109.40
2	A	701	ANP	N3-C2-N1	-5.14	120.64	128.68
2	C	701	ANP	O2G-PG-O1G	-4.75	101.52	113.45
2	C	701	ANP	C3'-C2'-C1'	4.54	107.81	100.98
2	C	701	ANP	O2G-PG-O3G	4.03	118.37	107.64
2	C	701	ANP	O1G-PG-N3B	-3.94	105.97	111.77
2	D	701	ANP	O2B-PB-O1B	3.61	117.49	109.92
2	A	701	ANP	C2'-C3'-C4'	-3.47	95.90	102.64
2	D	701	ANP	C3'-C2'-C1'	3.43	106.15	100.98
2	D	701	ANP	C4-C5-N7	-3.39	105.87	109.40
2	B	701	ANP	O2B-PB-O3A	3.25	115.50	104.64
2	B	701	ANP	O1B-PB-N3B	3.25	116.56	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	ANP	O2B-PB-O3A	2.85	114.15	104.64
2	A	701	ANP	O4'-C4'-C3'	2.85	110.75	105.11
2	D	701	ANP	C2-N1-C6	2.63	123.26	118.75
2	C	701	ANP	O2B-PB-O1B	2.60	115.38	109.92
2	C	701	ANP	O3A-PB-N3B	2.54	113.63	106.59
2	A	701	ANP	O1B-PB-N3B	-2.50	108.08	111.77
2	B	701	ANP	C2-N1-C6	2.50	123.03	118.75
2	A	701	ANP	C4-C5-N7	-2.46	106.83	109.40
2	B	701	ANP	C3'-C2'-C1'	2.44	104.66	100.98
2	C	701	ANP	C4-C5-N7	-2.43	106.87	109.40
2	B	701	ANP	O3A-PB-N3B	2.38	113.20	106.59
2	C	701	ANP	C2-N1-C6	2.34	122.76	118.75
2	C	701	ANP	C2'-C3'-C4'	-2.30	98.17	102.64
2	B	701	ANP	O4'-C1'-C2'	-2.20	103.71	106.93
2	D	701	ANP	O2G-PG-O1G	-2.09	108.19	113.45
2	B	701	ANP	O2G-PG-O3G	-2.09	102.07	107.64
2	D	701	ANP	O2G-PG-O3G	2.05	113.10	107.64
2	B	701	ANP	C5-C6-N6	2.01	123.40	120.35

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ANP	PB-N3B-PG-O1G
2	A	701	ANP	C5'-O5'-PA-O1A
2	A	701	ANP	C5'-O5'-PA-O2A
2	B	701	ANP	PB-N3B-PG-O1G
2	B	701	ANP	PG-N3B-PB-O1B
2	B	701	ANP	PB-O3A-PA-O5'
2	B	701	ANP	C5'-O5'-PA-O1A
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	C5'-O5'-PA-O1A
2	C	701	ANP	C5'-O5'-PA-O2A
2	D	701	ANP	PG-N3B-PB-O1B
2	D	701	ANP	PB-O3A-PA-O5'
2	D	701	ANP	C5'-O5'-PA-O1A
2	D	701	ANP	C5'-O5'-PA-O2A
3	A	702	MYR	C1-C2-C3-C4
3	D	702	MYR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	A	702	MYR	C7-C8-C9-C10
3	C	702	MYR	C10-C11-C12-C13
3	C	702	MYR	C3-C4-C5-C6
3	D	702	MYR	C6-C7-C8-C9
3	A	702	MYR	C2-C3-C4-C5
3	B	702	MYR	C3-C4-C5-C6
3	C	702	MYR	C11-C10-C9-C8
3	D	702	MYR	C11-C10-C9-C8
3	C	702	MYR	C2-C3-C4-C5
3	B	702	MYR	C10-C11-C12-C13
3	A	702	MYR	C11-C10-C9-C8
3	B	702	MYR	C7-C8-C9-C10
3	A	702	MYR	C10-C11-C12-C13
3	B	702	MYR	C11-C10-C9-C8
3	D	702	MYR	C3-C4-C5-C6
3	C	702	MYR	C6-C7-C8-C9
3	C	702	MYR	C4-C5-C6-C7
3	A	702	MYR	C11-C12-C13-C14
3	B	702	MYR	C11-C12-C13-C14
3	D	702	MYR	C7-C8-C9-C10
3	B	702	MYR	C4-C5-C6-C7
3	D	702	MYR	C4-C5-C6-C7
3	D	702	MYR	C2-C3-C4-C5
2	A	701	ANP	PB-O3A-PA-O5'
2	C	701	ANP	PB-O3A-PA-O5'
2	B	701	ANP	C5'-O5'-PA-O3A
2	C	701	ANP	C5'-O5'-PA-O3A
3	C	702	MYR	C9-C10-C11-C12
3	C	702	MYR	C7-C8-C9-C10
3	C	702	MYR	C11-C12-C13-C14
3	A	702	MYR	C3-C4-C5-C6
2	A	701	ANP	PB-O3A-PA-O2A
2	B	701	ANP	PB-O3A-PA-O2A
2	D	701	ANP	PB-O3A-PA-O2A
2	A	701	ANP	C5'-O5'-PA-O3A
2	D	701	ANP	C5'-O5'-PA-O3A

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	MYR	1	0

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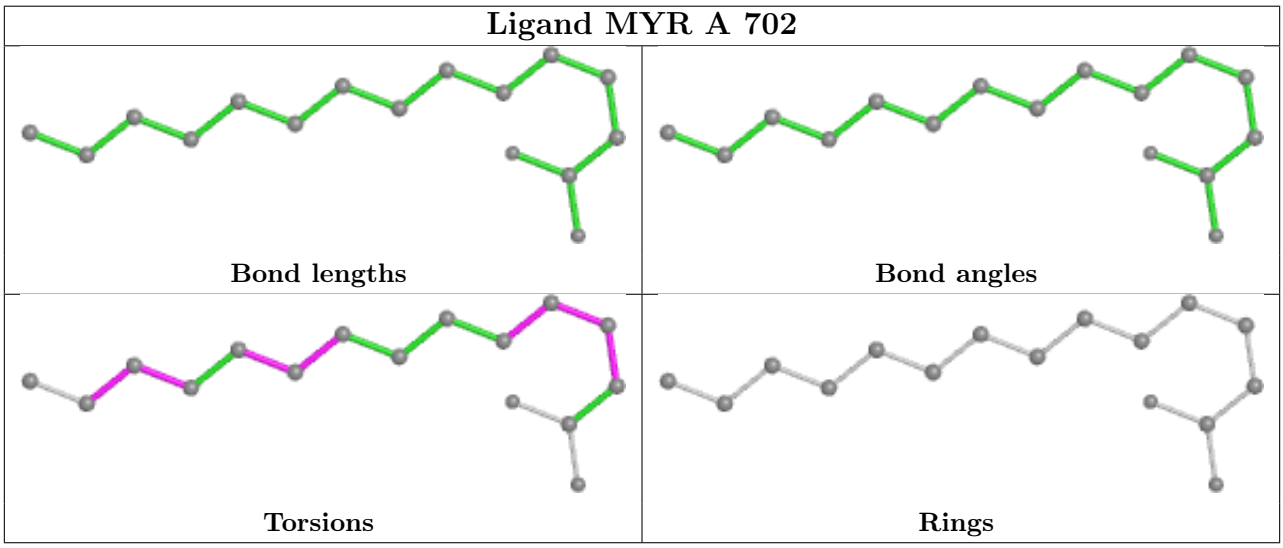
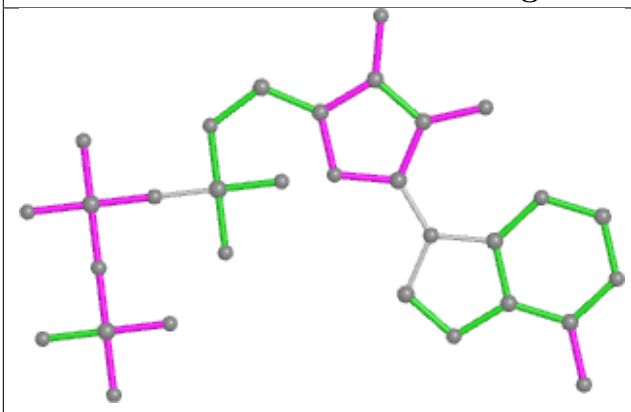
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ANP	1	0
2	D	701	ANP	1	0
3	B	702	MYR	1	0
2	B	701	ANP	1	0
3	C	702	MYR	5	0
3	D	702	MYR	1	0
2	C	701	ANP	3	0

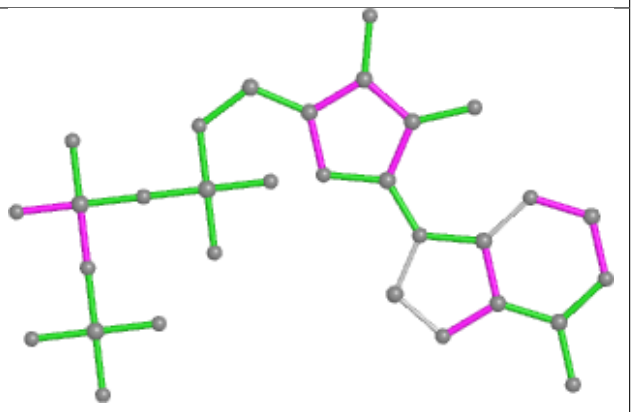
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



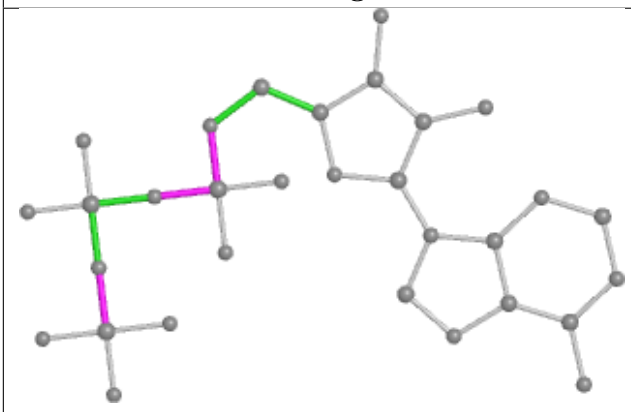
Ligand ANP A 701



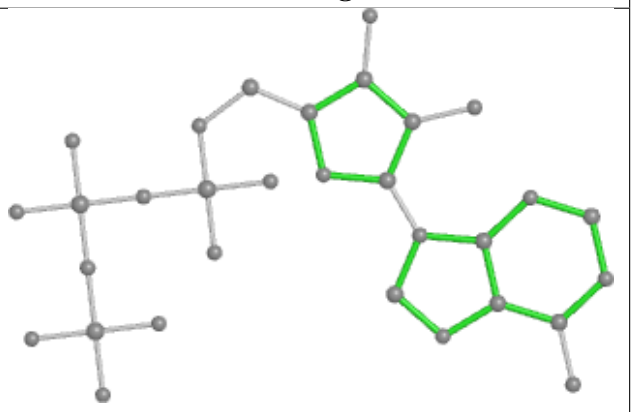
Bond lengths



Bond angles

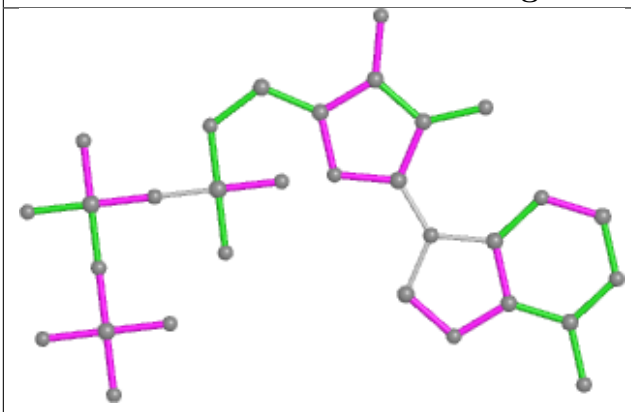


Torsions

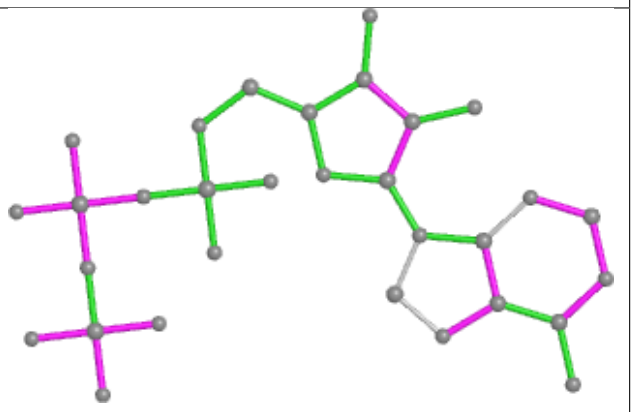


Rings

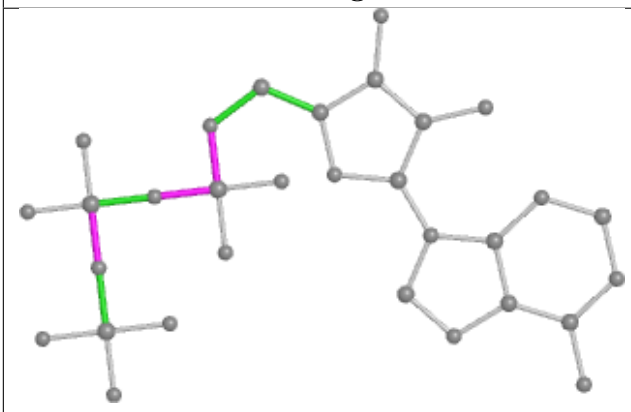
Ligand ANP D 701



Bond lengths



Bond angles



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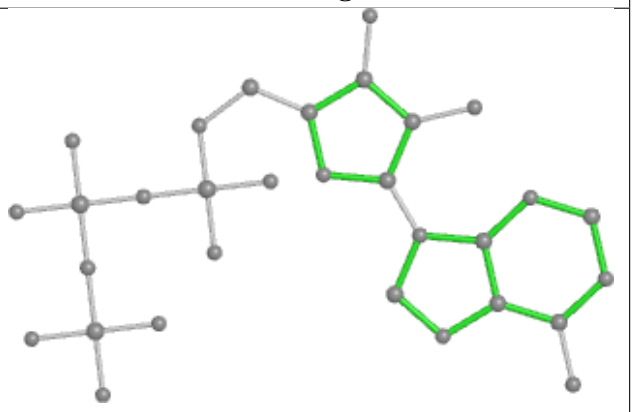
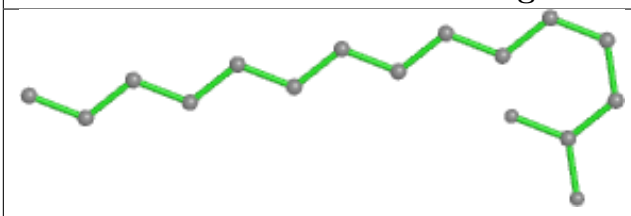
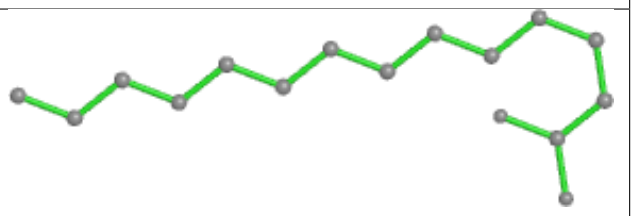


Rings

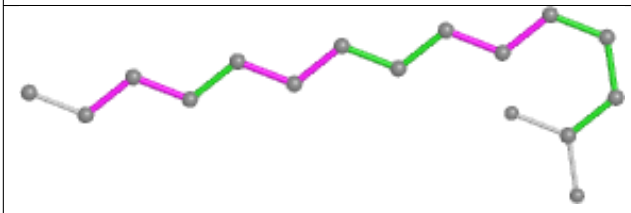
Ligand MYR B 702



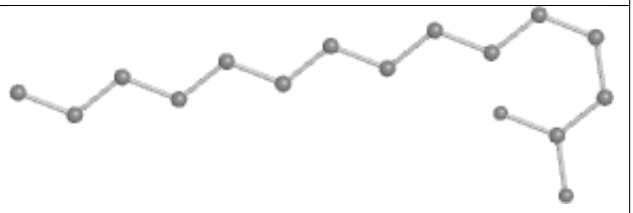
Bond lengths



Bond angles

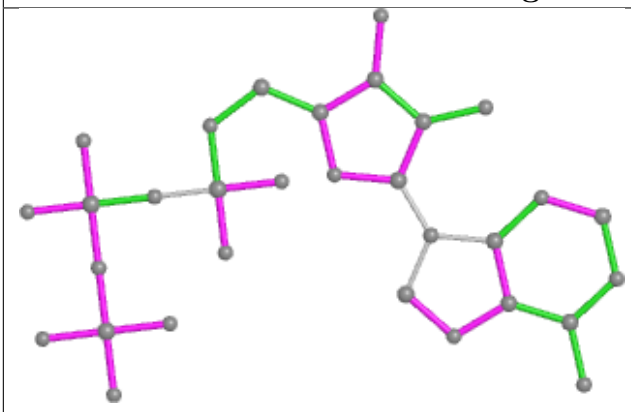


Torsions

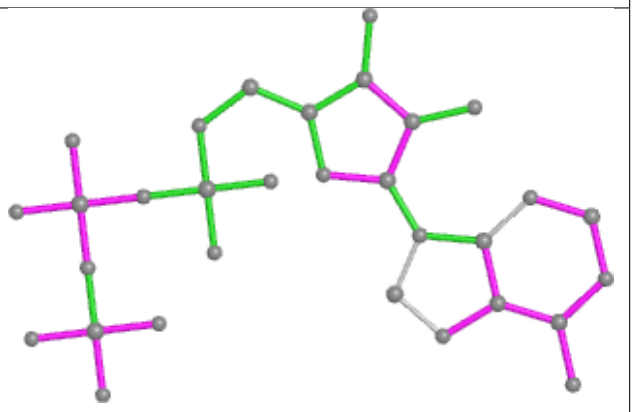


Rings

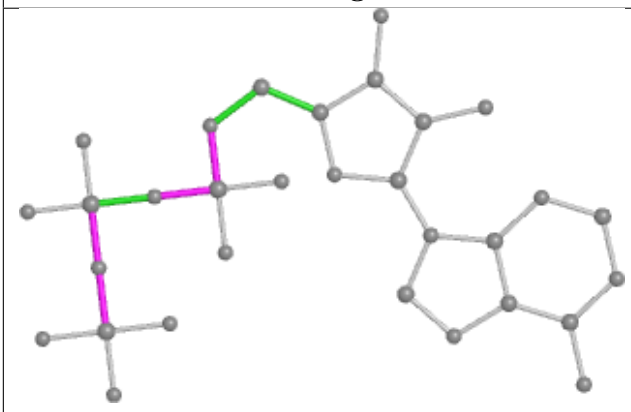
Ligand ANP B 701



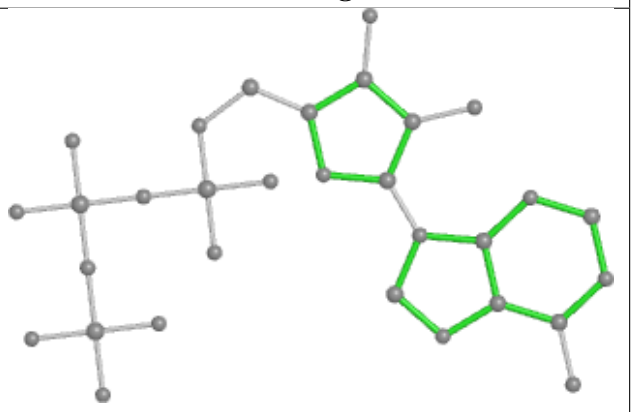
Bond lengths



Bond angles

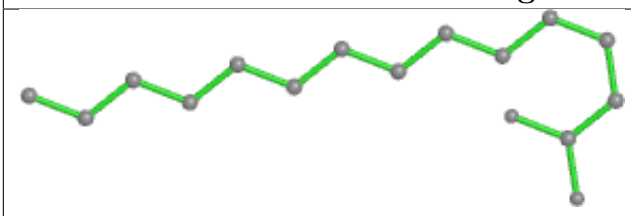


Torsions

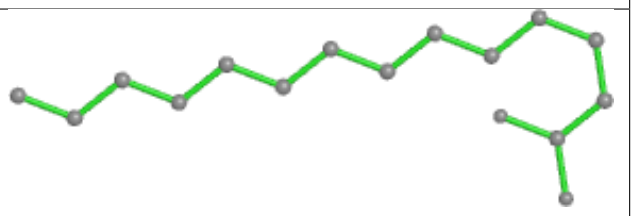


Rings

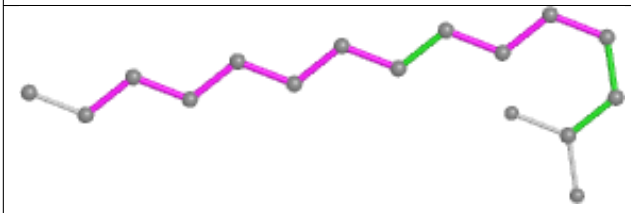
Ligand MYR C 702



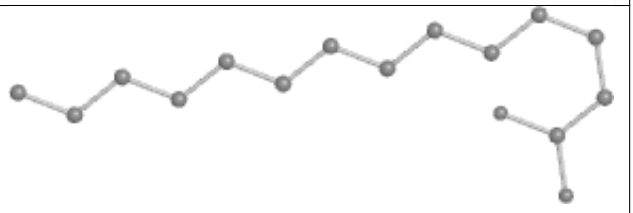
Bond lengths



Bond angles

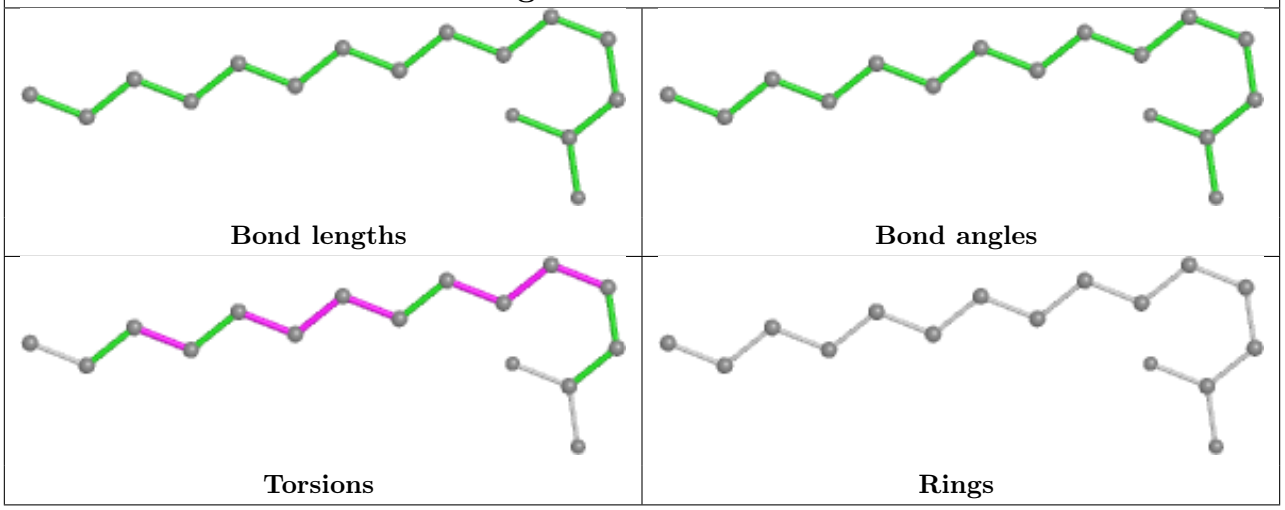


Torsions

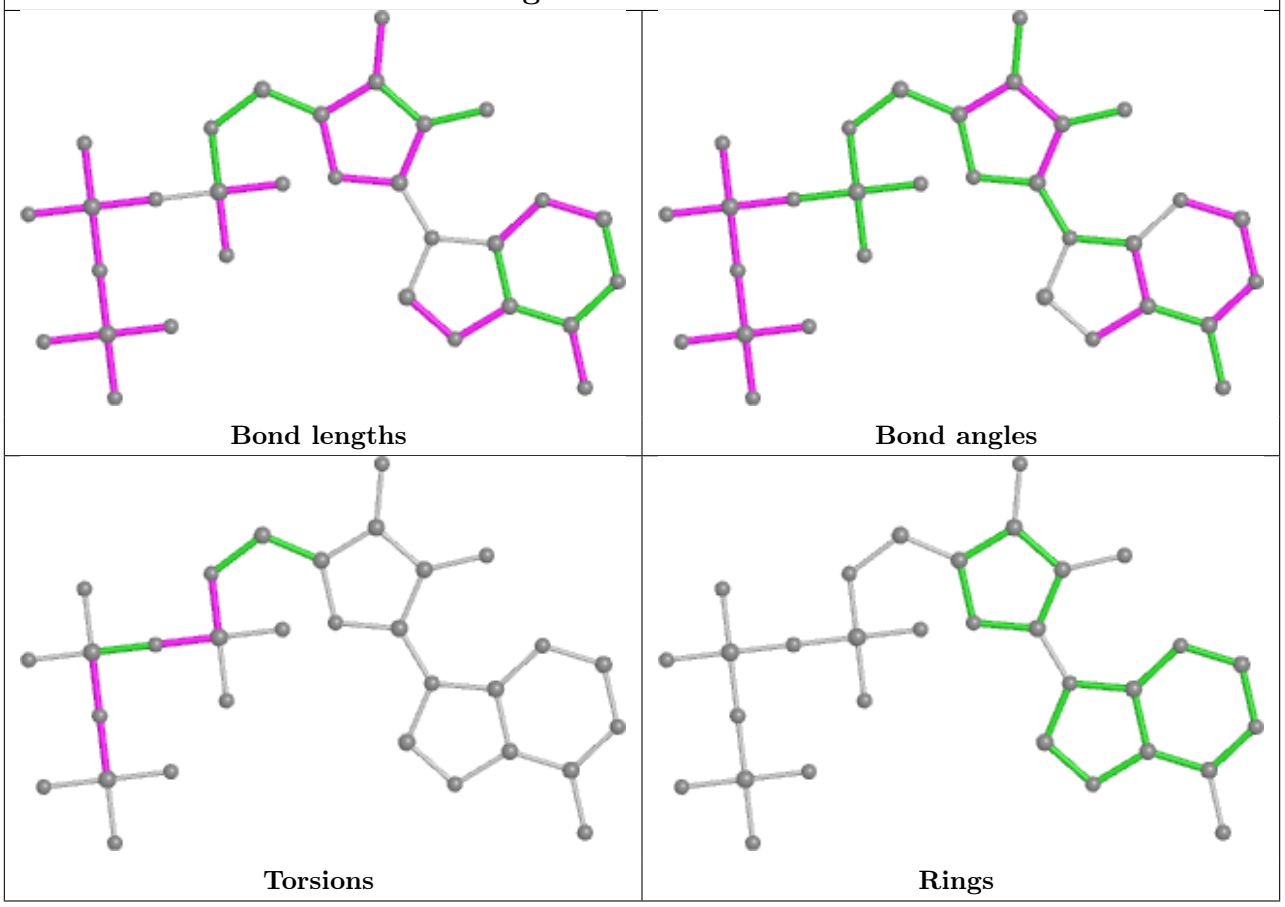


Rings

Ligand MYR D 702



Ligand ANP C 701



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, 95^{th} 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	603/604 (99%)	0.33	25 (4%) 37 36	10, 22, 44, 69	0
1	B	597/604 (98%)	0.52	54 (9%) 9 8	12, 29, 54, 80	0
1	C	593/604 (98%)	0.66	66 (11%) 5 4	10, 26, 55, 75	0
1	D	490/604 (81%)	0.31	25 (5%) 28 27	11, 22, 47, 65	0
All	All	2283/2416 (94%)	0.46	170 (7%) 14 13	10, 25, 51, 80	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	584	LEU	12.6
1	A	534	ALA	12.5
1	D	496	LEU	12.5
1	C	589	GLY	12.3
1	C	588	SER	11.8
1	C	595	VAL	11.6
1	A	186	ALA	9.7
1	A	184	ALA	9.6
1	A	535	VAL	9.5
1	A	533	ASP	7.7
1	C	586	SER	7.5
1	C	591	ILE	7.5
1	A	13	ALA	7.5
1	C	599	ALA	7.4
1	C	585	ARG	7.2
1	C	583	ILE	6.6
1	C	579	ALA	6.6
1	C	598	LYS	6.4
1	C	546	LEU	6.0
1	C	3	LEU	5.9
1	C	582	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	562	ALA	5.1
1	A	185	ALA	5.0
1	B	530	ILE	4.9
1	A	14	LYS	4.8
1	C	596	ASN	4.8
1	C	531	GLU	4.8
1	A	15	GLY	4.7
1	B	500	ALA	4.7
1	A	532	GLY	4.7
1	C	587	SER	4.6
1	B	122	ALA	4.6
1	D	495	ASP	4.6
1	C	594	ARG	4.6
1	C	549	ASP	4.6
1	C	37	VAL	4.5
1	C	520	ILE	4.5
1	B	284	GLU	4.4
1	C	590	LYS	4.4
1	B	392	ASP	4.4
1	C	535	VAL	4.4
1	C	120	GLY	4.3
1	B	570	VAL	4.3
1	B	573	ALA	4.3
1	D	13	ALA	4.3
1	A	285	GLY	4.2
1	A	8	GLY	4.1
1	B	564	VAL	4.1
1	B	13	ALA	4.1
1	B	178	ILE	4.0
1	C	13	ALA	4.0
1	C	534	ALA	4.0
1	B	563	ALA	3.9
1	C	533	ASP	3.9
1	C	593	ARG	3.8
1	B	285	GLY	3.7
1	A	284	GLU	3.7
1	B	571	VAL	3.7
1	B	531	GLU	3.6
1	D	285	GLY	3.5
1	B	566	GLU	3.5
1	C	392	ASP	3.4
1	B	559	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	578	VAL	3.4
1	D	460	ASN	3.4
1	B	460	ASN	3.4
1	C	547	ASP	3.4
1	A	604	HIS	3.3
1	B	120	GLY	3.3
1	B	558	ASP	3.3
1	D	391	GLY	3.3
1	C	597	LYS	3.3
1	B	286	ASP	3.3
1	D	309	GLU	3.3
1	C	525	VAL	3.3
1	B	308	SER	3.3
1	C	580	PRO	3.3
1	D	393	ASN	3.3
1	B	499	ILE	3.2
1	D	14	LYS	3.2
1	D	392	ASP	3.2
1	B	569	GLY	3.1
1	B	181	PRO	3.1
1	B	574	ASP	3.1
1	B	561	ARG	3.0
1	B	56	VAL	3.0
1	B	501	GLY	3.0
1	D	3	LEU	2.9
1	B	567	ALA	2.9
1	B	502	ARG	2.9
1	D	38	ASP	2.9
1	C	501	GLY	2.8
1	C	550	PRO	2.8
1	C	524	ALA	2.8
1	C	529	ALA	2.8
1	C	592	ALA	2.8
1	B	15	GLY	2.8
1	C	38	ASP	2.7
1	C	518	GLU	2.7
1	D	378	GLU	2.7
1	B	200	THR	2.7
1	B	393	ASN	2.7
1	D	37	VAL	2.7
1	A	392	ASP	2.7
1	A	53	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	555	GLU	2.6
1	B	248	ILE	2.6
1	B	537	GLN	2.6
1	D	382	ALA	2.6
1	D	284	GLU	2.6
1	B	551	SER	2.6
1	B	310	GLY	2.6
1	C	523	ALA	2.6
1	B	5	LYS	2.5
1	A	248	ILE	2.5
1	C	182	SER	2.5
1	C	460	ASN	2.5
1	C	233	PRO	2.5
1	C	522	PRO	2.5
1	C	528	PHE	2.5
1	C	576	ARG	2.5
1	D	459	GLU	2.5
1	C	530	ILE	2.5
1	B	511	TYR	2.5
1	D	233	PRO	2.4
1	B	309	GLU	2.4
1	D	5	LYS	2.4
1	B	53	GLU	2.4
1	B	565	THR	2.4
1	A	310	GLY	2.4
1	A	37	VAL	2.4
1	A	56	VAL	2.4
1	B	179	PRO	2.4
1	B	572	PRO	2.4
1	D	414	PRO	2.4
1	D	493	LEU	2.3
1	A	11	PHE	2.3
1	A	12	ASP	2.3
1	B	560	ILE	2.3
1	C	459	GLU	2.3
1	A	308	SER	2.3
1	C	515	HIS	2.3
1	C	581	ASP	2.3
1	C	511	TYR	2.3
1	B	575	ILE	2.3
1	C	551	SER	2.3
1	A	114	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	384	ARG	2.3
1	D	381	ALA	2.2
1	C	54	GLY	2.2
1	C	548	ARG	2.2
1	C	12	ASP	2.2
1	B	204	THR	2.2
1	C	5	LYS	2.2
1	C	118	GLU	2.1
1	C	242	LEU	2.1
1	D	418	THR	2.1
1	B	287	ASN	2.1
1	C	543	GLU	2.1
1	A	16	ASN	2.1
1	C	532	GLY	2.1
1	C	484	ASP	2.1
1	B	4	HIS	2.1
1	B	518	GLU	2.1
1	C	285	GLY	2.1
1	C	200	THR	2.0
1	B	516	ALA	2.0
1	C	566	GLU	2.0
1	B	504	HIS	2.0
1	D	415	GLU	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, 95^{th} 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.

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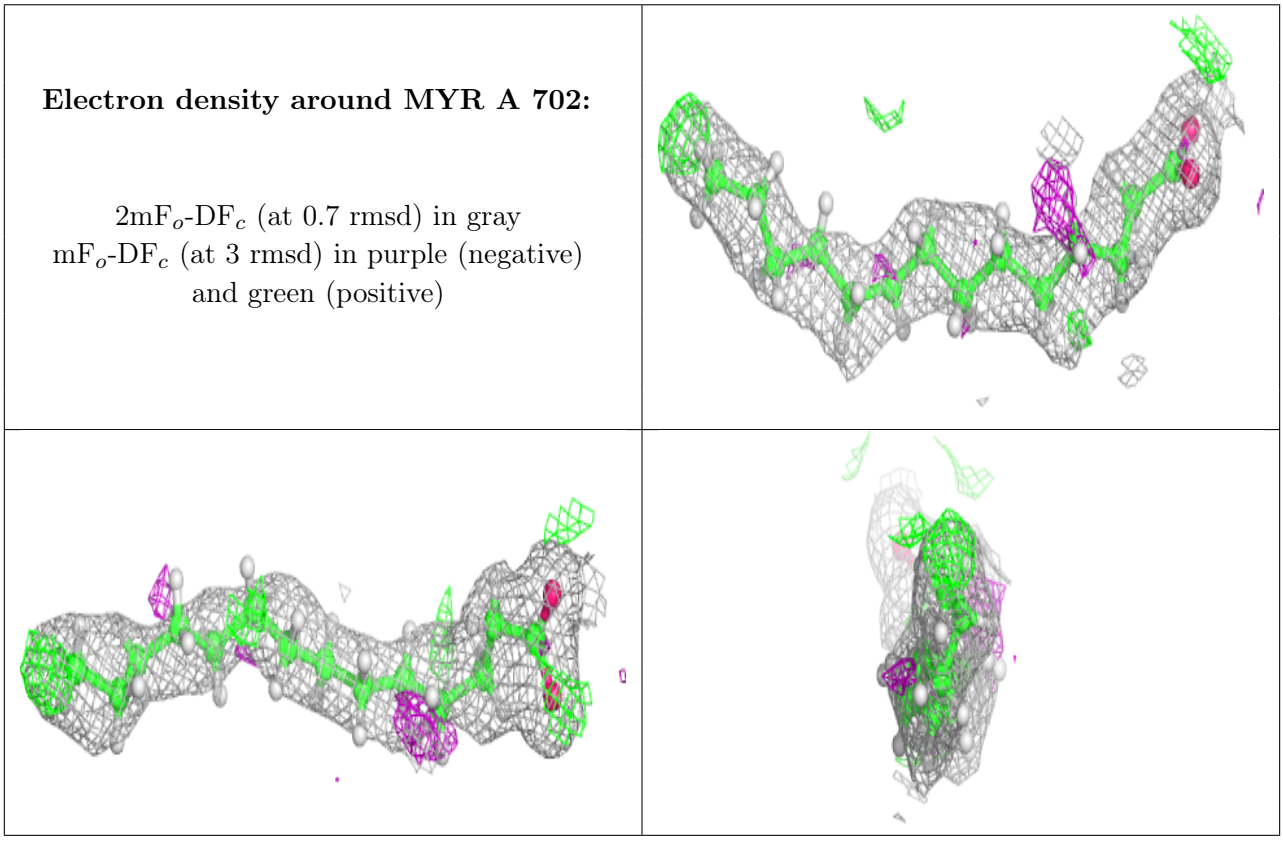
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	703	1/1	0.58	0.16	30,30,30,30	0
4	MG	A	703	1/1	0.64	0.14	30,30,30,30	0
3	MYR	A	702	16/16	0.87	0.18	19,37,48,50	0
2	ANP	C	701	31/31	0.90	0.15	17,26,70,93	0
3	MYR	D	702	16/16	0.90	0.13	21,31,44,46	0
3	MYR	C	702	16/16	0.91	0.14	25,35,46,50	0
3	MYR	B	702	16/16	0.91	0.13	20,35,49,55	0
2	ANP	D	701	31/31	0.92	0.14	16,23,66,101	0
2	ANP	B	701	31/31	0.94	0.11	12,21,47,66	0
2	ANP	A	701	31/31	0.96	0.10	9,17,29,32	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.

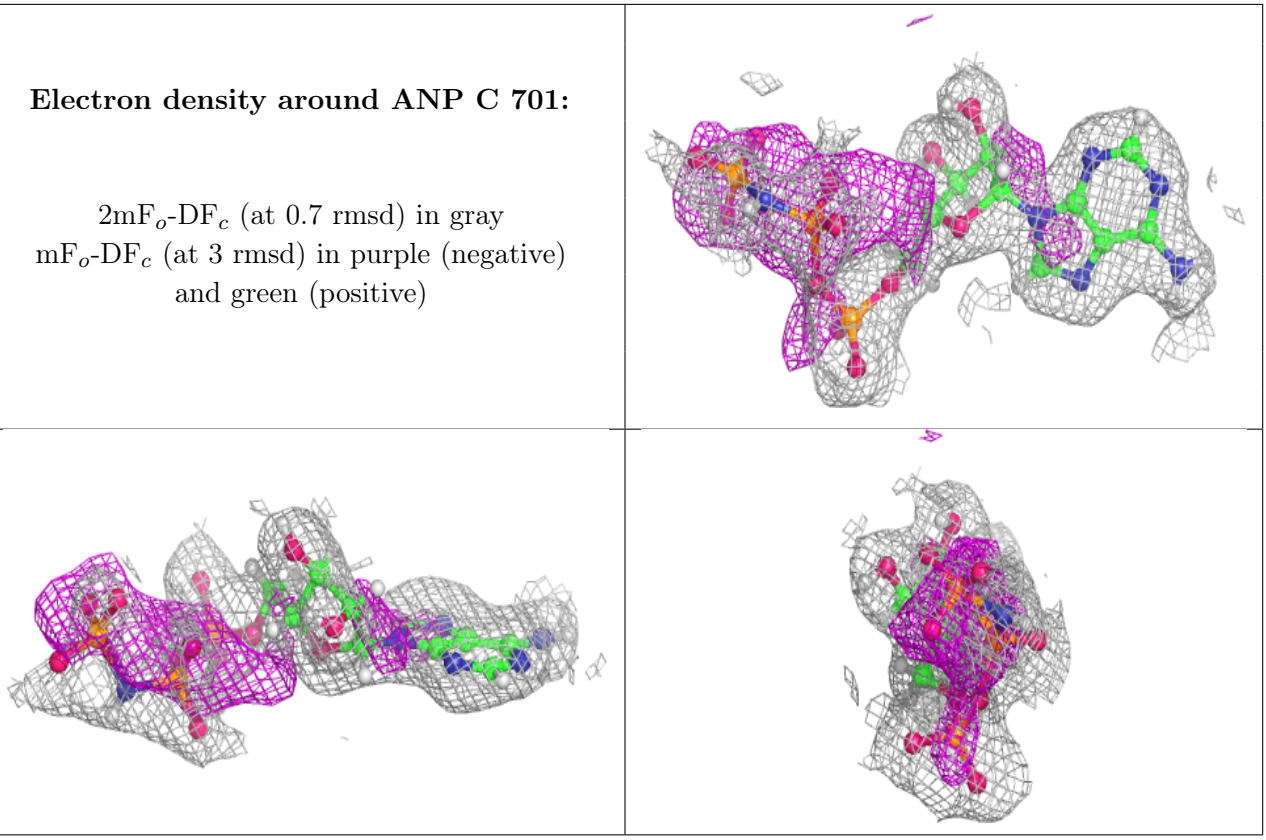
Electron density around MYR A 702:

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



Electron density around 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 MYR D 702:

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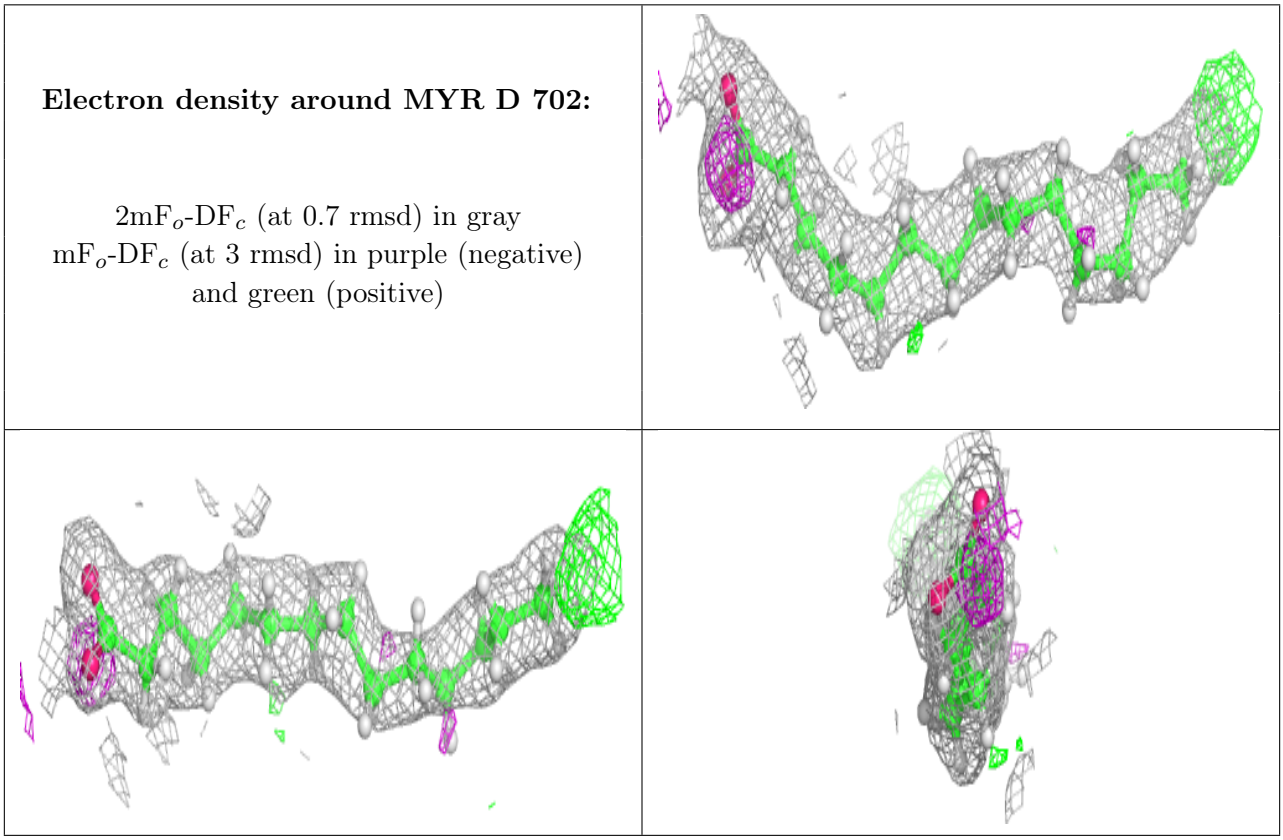
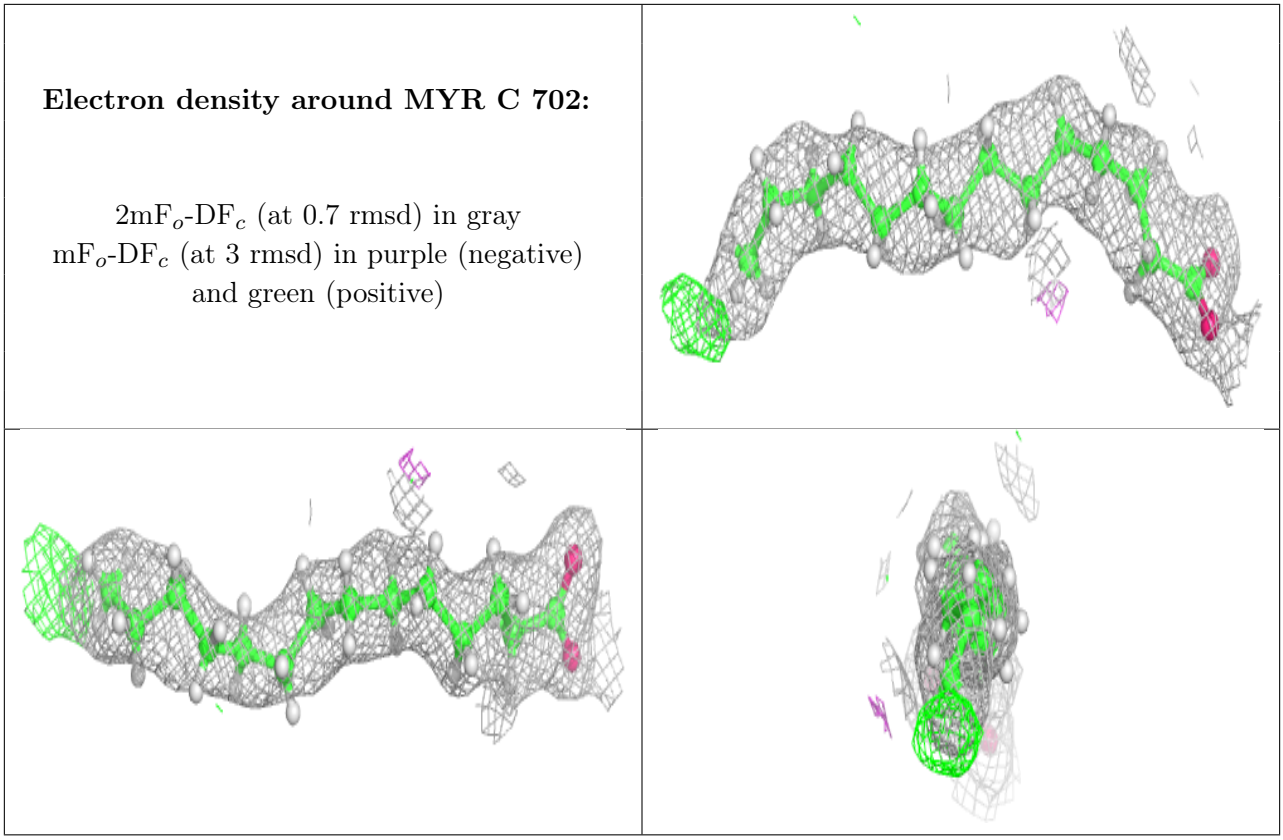
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



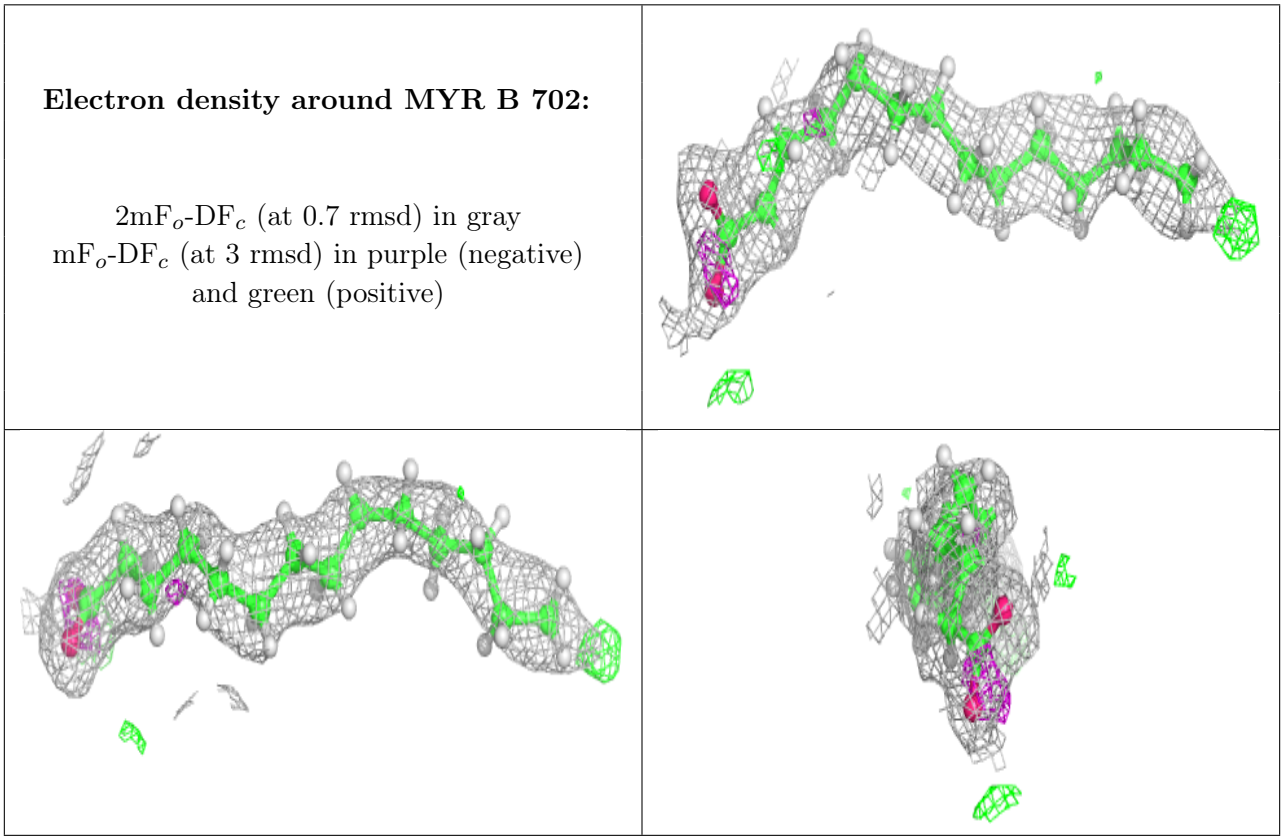
Electron density around MYR C 702:

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



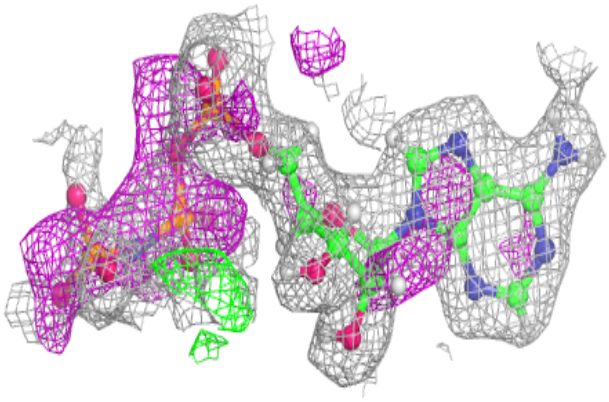
Electron density around MYR B 702:

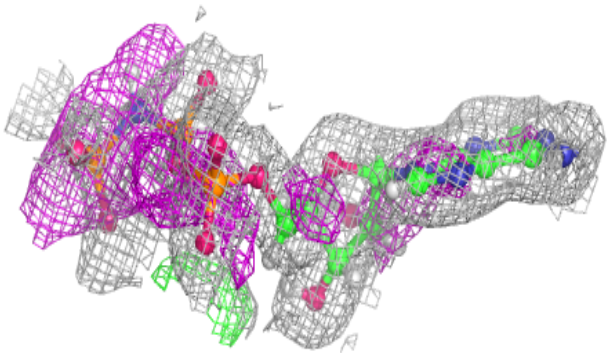
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

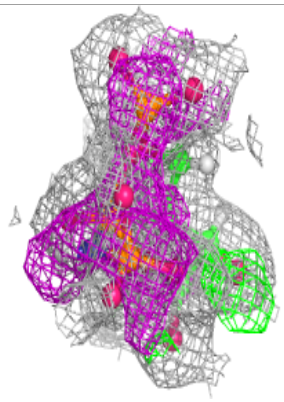


Electron density around ANP D 701:

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

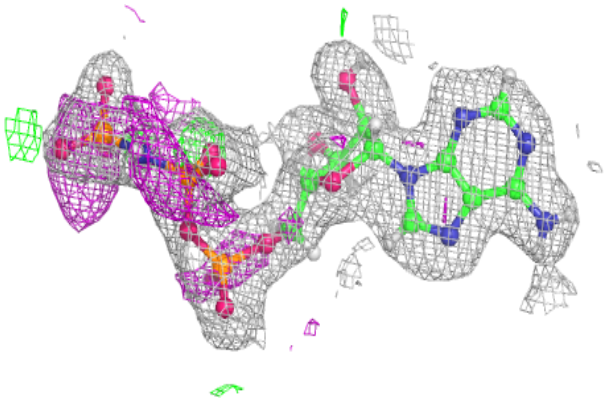


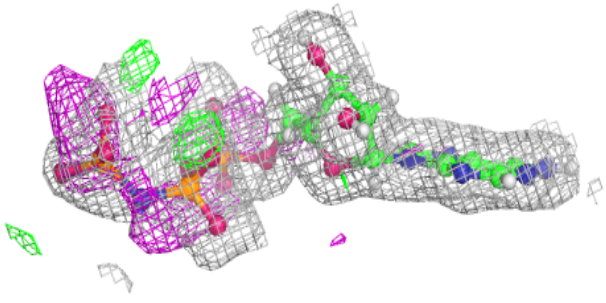


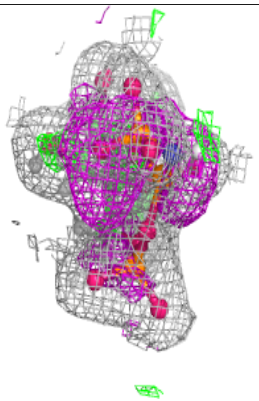


Electron density around ANP B 701:

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

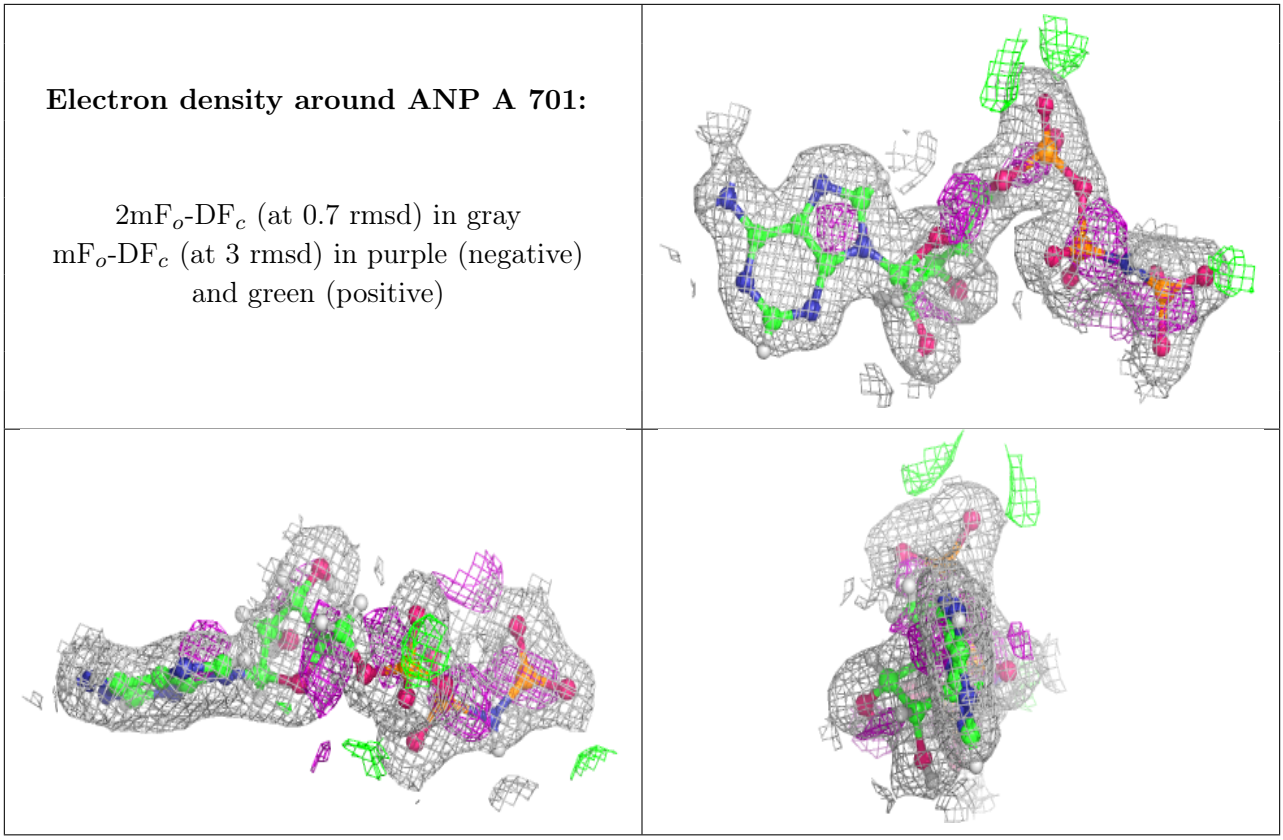






Electron density around ANP A 701:

$2mF_o$-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.