



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:28 AM UTC

PDB ID : 7WUA / pdb_00007wua
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

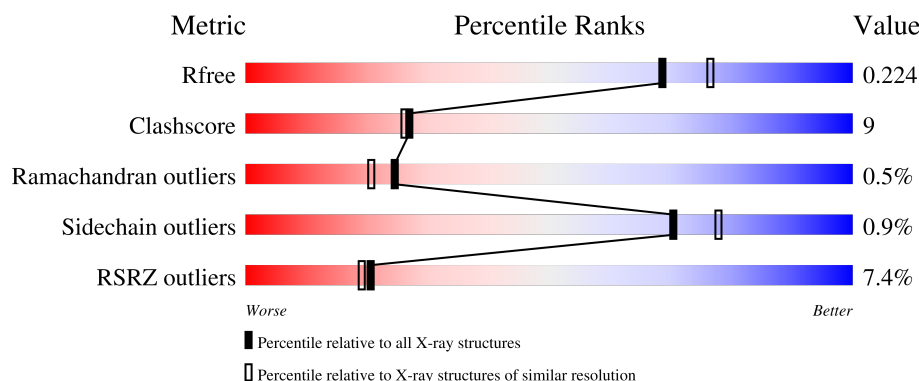
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	604	4% 87% 12%
1	B	604	8% 79% 20% .
1	C	604	11% 77% 19% ...
1	D	604	4% 69% 12% 19%

2 Entry composition

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:

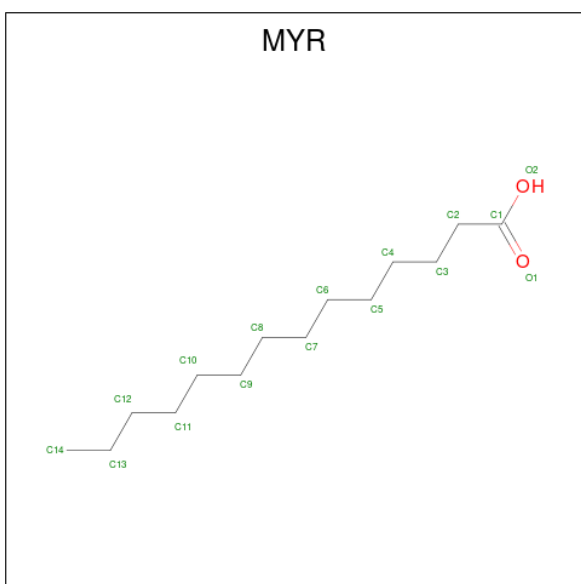
Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ILE	VAL	conflict	UNP A0A679LZK7
B	254	ILE	VAL	conflict	UNP A0A679LZK7
C	254	ILE	VAL	conflict	UNP A0A679LZK7
D	254	ILE	VAL	conflict	UNP A0A679LZK7

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 3 is MYRISTIC ACID (CCD ID: 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 43	C 14	H 27	O 2	0	0
3	B	1	Total 43	C 14	H 27	O 2	0	0
3	C	1	Total 43	C 14	H 27	O 2	0	0
3	D	1	Total 43	C 14	H 27	O 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

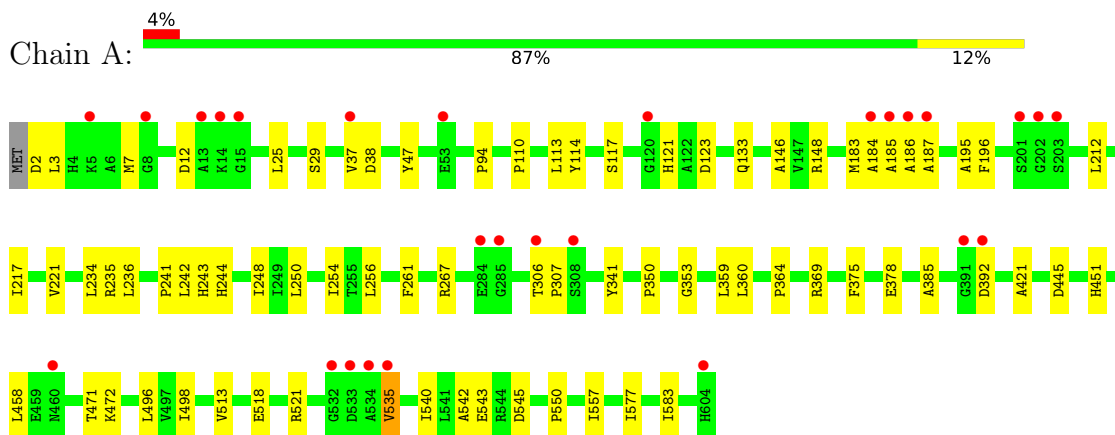
- Molecule 5 is water.

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

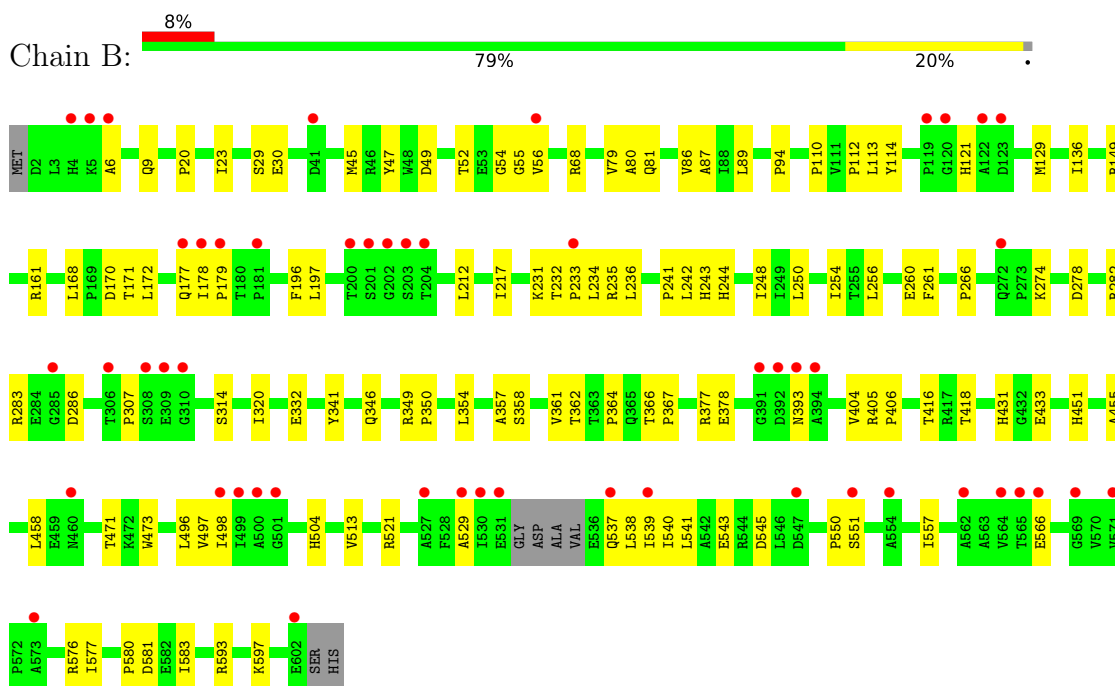
3 Residue-property plots

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



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4 Data and refinement statistics

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 46.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (46.10-2.00) 97.2 (46.10-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.185 , 0.224 0.188 , 0.224	Depositor DCC
R_{free} test set	9564 reflections (4.80%)	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 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, MYR

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	0.33	1/4715 (0.0%)	0.52	3/6432 (0.0%)
1	B	0.23	1/4673 (0.0%)	0.40	0/6373
1	C	0.42	4/4625 (0.1%)	0.66	15/6311 (0.2%)
1	D	0.28	1/3840 (0.0%)	0.46	0/5241
All	All	0.33	7/17853 (0.0%)	0.52	18/24357 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	PRO	C-O	-7.39	1.14	1.23
1	A	550	PRO	C-O	-6.68	1.15	1.24
1	C	186	ALA	C-O	-6.26	1.16	1.24
1	B	550	PRO	C-O	-5.38	1.17	1.24
1	D	207	PRO	C-O	-5.35	1.17	1.23
1	C	185	ALA	C-O	-5.25	1.17	1.24
1	C	187	ALA	C-O	-5.02	1.16	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	586	SER	CA-C-N	7.48	135.82	121.54
1	C	586	SER	C-N-CA	7.48	135.82	121.54
1	C	591	ILE	CA-C-O	-7.08	113.66	121.23
1	C	592	ALA	CA-C-N	6.50	133.95	121.54
1	C	592	ALA	C-N-CA	6.50	133.95	121.54
1	C	596	ASN	CA-C-N	6.50	133.95	121.54
1	C	596	ASN	C-N-CA	6.50	133.95	121.54
1	C	593	ARG	CA-C-N	6.12	133.22	121.54
1	C	593	ARG	C-N-CA	6.12	133.22	121.54
1	C	523	ALA	CA-C-N	-6.11	113.57	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	523	ALA	C-N-CA	-6.11	113.57	122.06
1	A	186	ALA	O-C-N	6.00	128.50	122.08
1	A	186	ALA	CA-C-N	5.98	132.97	121.54
1	A	186	ALA	C-N-CA	5.98	132.97	121.54
1	C	581	ASP	CB-CA-C	-5.59	102.45	111.28
1	C	593	ARG	N-CA-CB	5.42	119.64	110.49
1	C	581	ASP	O-C-N	5.40	129.43	122.20
1	C	586	SER	O-C-N	5.00	129.24	122.59

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	58	0
1	B	4578	0	4532	89	0
1	C	4531	0	4482	110	0
1	D	3758	0	3718	62	0
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	21	0
5	B	421	0	0	14	0
5	C	482	0	0	17	0
5	D	441	0	0	14	0
All	All	19608	160	17454	324	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 (324) 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
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

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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	0.70
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
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:539:ILE:HD12	1:C:597:LYS:HZ2	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
5:A:953:HOH:O	1:D:183:MET:HE3	2.01	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
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:A:234:LEU:HD12	1:A:234:LEU:C	2.31	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:C:444:GLU:HG2	1:C:445:ASP:N	2.20	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:A:472:LYS:NZ	5:A:814:HOH:O	2.30	0.55
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:D:262:GLU:CD	1:D:283:ARG:HH22	2.13	0.55
1:C:521:ARG:HH12	1:C:580:PRO:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:594:ARG:HG2	1:C:598:LYS:HZ1	1.73	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: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: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:B:451:HIS:HA	1:B:471:THR:O	2.09	0.52
1:C:30:GLU:OE2	1:C:70:LYS:NZ	2.41	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: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
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:4:HIS:HB2	1:C:5:LYS:HZ1	1.76	0.51
1:C:303:ARG:HD2	1:C:304:TYR:CZ	2.46	0.51
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:D:496:LEU:C	1:D:496:LEU:CD2	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:LEU:O	1:C:442:ARG:HG3	2.12	0.49
1:B:529:ALA:O	1:B:597:LYS:NZ	2.31	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:C:232:THR:HA	1:C:233:PRO:C	2.38	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
1:D:469:GLU:N	1:D:469:GLU:OE1	2.47	0.47
1:C:444:GLU:CD	1:C:444:GLU:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:234:LEU:C	1:B:234:LEU:HD12	2.40	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:539:ILE:HD12	1:C:597:LYS:HZ1	1.78	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:C:125:LEU:HD11	1:C:129:MET:HE3	1.98	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:B:87:ALA:CB	1:B:129:MET:HE1	2.47	0.45
1:C:495:ASP:OD2	1:C:593:ARG:NH2	2.47	0.45
1:D:469:GLU:H	1:D:469:GLU:CD	2.25	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:507:GLN:HG2	1:C:508:ASP:N	2.32	0.44
1:D:492:ARG:HH22	1:D:494:LYS:HE2	1.79	0.44
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:30:GLU:OE1	1:B:30:GLU:HA	2.17	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:234:LEU:C	1:C:234:LEU:HD12	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:87:ALA:CB	1:C:129:MET:HE1	2.48	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:H	1:C:598:LYS:HG3	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: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
1:C:583:ILE:CD1	1:C:595:VAL:CG1	2.93	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: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:B:232:THR:HA	1:B:233:PRO:C	2.45	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:7:MET:HE1	1:A:221:VAL:HG12	2.02	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:A:12:ASP:C	1:A:12:ASP:OD1	2.63	0.41
1:C:543:GLU:OE2	1:C:581:ASP:N	2.54	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:B:538:LEU:C	1:B:539:ILE:HD13	2.46	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
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:C:594:ARG:HE	1:C:598:LYS:HZ1	1.69	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%)	18	14
1	B	593/604 (98%)	577 (97%)	16 (3%)	0	100	100
1	C	589/604 (98%)	557 (95%)	25 (4%)	7 (1%)	10	6
1	D	486/604 (80%)	473 (97%)	13 (3%)	0	100	100
All	All	2269/2416 (94%)	2190 (96%)	68 (3%)	11 (0%)	24	21

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
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%)	480 (100%)	2 (0%)	84	89
1	B	478/483 (99%)	478 (100%)	0	100	100
1	C	471/483 (98%)	459 (98%)	12 (2%)	42	45
1	D	394/483 (82%)	392 (100%)	2 (0%)	81	87
All	All	1825/1932 (94%)	1809 (99%)	16 (1%)	70	78

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

Mol	Chain	Res	Type
1	A	183	MET
1	A	369	ARG
1	C	183	MET
1	C	274	LYS
1	C	369	ARG
1	C	549	ASP
1	C	582	GLU
1	C	586	SER
1	C	591	ILE
1	C	593	ARG
1	C	594	ARG
1	C	595	VAL
1	C	597	LYS
1	C	598	LYS
1	D	274	LYS
1	D	496	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	287	ASN
1	A	365	GLN
1	A	507	GLN
1	B	81	GLN
1	B	365	GLN
1	B	393	ASN
1	B	460	ASN
1	B	515	HIS
1	B	537	GLN
1	C	81	GLN

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Mol	Chain	Res	Type
1	C	158	GLN
1	C	198	GLN
1	C	243	HIS
1	C	287	ASN
1	C	365	GLN
1	C	460	ASN
1	D	16	ASN
1	D	244	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
2	ANP	B	701	4	33,33,33	4.73	22 (66%)	45,52,52	2.93	15 (33%)
3	MYR	D	702	-	15,15,15	0.61	0	15,15,15	0.77	0
2	ANP	C	701	-	33,33,33	4.19	23 (69%)	45,52,52	2.72	17 (37%)
2	ANP	D	701	-	33,33,33	3.59	20 (60%)	45,52,52	2.98	16 (35%)
3	MYR	B	702	-	15,15,15	0.61	0	15,15,15	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MYR	A	702	-	15,15,15	0.64	0	15,15,15	0.77	0
2	ANP	A	701	4	33,33,33	3.45	17 (51%)	45,52,52	2.08	13 (28%)
3	MYR	C	702	-	15,15,15	0.60	0	15,15,15	0.67	0

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	B	701	4	-	8/18/38/38	0/3/3/3
3	MYR	D	702	-	-	7/13/13/13	-
2	ANP	C	701	-	-	8/18/38/38	0/3/3/3
2	ANP	D	701	-	-	7/18/38/38	0/3/3/3
3	MYR	B	702	-	-	6/13/13/13	-
3	MYR	A	702	-	-	7/13/13/13	-
2	ANP	A	701	4	-	7/18/38/38	0/3/3/3
3	MYR	C	702	-	-	9/13/13/13	-

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ANP	PB-O1B	-10.37	1.30	1.46
2	A	701	ANP	O4'-C1'	10.31	1.65	1.42
2	B	701	ANP	O4'-C1'	10.12	1.65	1.42
2	B	701	ANP	O4'-C4'	-9.49	1.23	1.45
2	D	701	ANP	O4'-C1'	8.94	1.62	1.42
2	C	701	ANP	O4'-C1'	8.65	1.62	1.42
2	D	701	ANP	O4'-C4'	-8.41	1.26	1.45
2	C	701	ANP	O4'-C4'	-8.25	1.26	1.45
2	C	701	ANP	PB-O3A	8.17	1.69	1.59
2	B	701	ANP	PG-O3G	-7.65	1.36	1.56
2	B	701	ANP	PG-O1G	-7.53	1.34	1.46
2	D	701	ANP	O3'-C3'	-6.85	1.26	1.43
2	B	701	ANP	O3'-C3'	-6.64	1.26	1.43
2	C	701	ANP	O3'-C3'	-6.61	1.26	1.43
2	C	701	ANP	PG-N3B	6.44	1.80	1.63
2	D	701	ANP	PB-O2B	-6.20	1.40	1.56
2	A	701	ANP	O4'-C4'	-6.10	1.31	1.45
2	B	701	ANP	C8-N9	-5.92	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ANP	PB-O3A	5.83	1.66	1.59
2	A	701	ANP	PG-N3B	5.70	1.78	1.63
2	B	701	ANP	PB-O2B	-5.58	1.42	1.56
2	C	701	ANP	PG-O1G	-5.57	1.37	1.46
2	B	701	ANP	PG-O2G	-5.48	1.42	1.56
2	C	701	ANP	C2'-C1'	-5.39	1.36	1.53
2	D	701	ANP	C2'-C1'	-5.23	1.37	1.53
2	A	701	ANP	C2'-C1'	-5.19	1.37	1.53
2	C	701	ANP	PB-O2B	-5.04	1.43	1.56
2	A	701	ANP	O3'-C3'	-4.90	1.30	1.43
2	B	701	ANP	C2'-C1'	-4.85	1.38	1.53
2	D	701	ANP	C8-N9	-4.75	1.29	1.37
2	B	701	ANP	PA-O3A	-4.73	1.54	1.59
2	C	701	ANP	C5-N7	-4.72	1.30	1.39
2	B	701	ANP	C5-N7	-4.68	1.30	1.39
2	B	701	ANP	PG-N3B	4.55	1.75	1.63
2	A	701	ANP	C3'-C4'	4.37	1.64	1.53
2	D	701	ANP	C5-N7	-4.14	1.31	1.39
2	C	701	ANP	PG-O3G	-4.09	1.45	1.56
2	C	701	ANP	C2-N3	-4.09	1.26	1.33
2	C	701	ANP	PG-O2G	-4.07	1.46	1.56
2	B	701	ANP	PA-O2A	-4.03	1.36	1.55
2	D	701	ANP	PA-O2A	-3.82	1.37	1.55
2	C	701	ANP	C3'-C4'	3.72	1.62	1.53
2	D	701	ANP	C3'-C4'	3.68	1.62	1.53
2	D	701	ANP	C1'-N9	-3.64	1.36	1.46
2	C	701	ANP	C4-N9	-3.64	1.30	1.37
2	C	701	ANP	PA-O2A	-3.61	1.38	1.55
2	C	701	ANP	C8-N9	-3.48	1.31	1.37
2	A	701	ANP	PG-O3G	-3.45	1.47	1.56
2	D	701	ANP	C2-N3	-3.41	1.27	1.33
2	B	701	ANP	C3'-C4'	3.35	1.61	1.53
2	C	701	ANP	PA-O3A	3.32	1.63	1.59
2	A	701	ANP	PB-O2B	-3.29	1.48	1.56
2	C	701	ANP	C1'-N9	-3.28	1.37	1.46
2	A	701	ANP	O2'-C2'	3.24	1.51	1.43
2	A	701	ANP	PB-N3B	3.24	1.71	1.63
2	A	701	ANP	C6-N6	3.21	1.42	1.34
2	B	701	ANP	C1'-N9	-3.20	1.37	1.46
2	C	701	ANP	PB-O1B	-3.16	1.41	1.46
2	B	701	ANP	C2-N3	-3.13	1.28	1.33
2	D	701	ANP	PG-N3B	3.08	1.71	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ANP	C4-N9	-3.05	1.31	1.37
2	A	701	ANP	PA-O3A	2.99	1.62	1.59
2	D	701	ANP	PG-O2G	-2.98	1.48	1.56
2	A	701	ANP	PB-O1B	2.93	1.50	1.46
2	A	701	ANP	C1'-N9	-2.92	1.38	1.46
2	C	701	ANP	PB-N3B	2.86	1.70	1.63
2	D	701	ANP	PG-O1G	-2.79	1.42	1.46
2	C	701	ANP	C6-N6	2.79	1.41	1.34
2	B	701	ANP	C5-C4	-2.75	1.34	1.39
2	D	701	ANP	PB-O3A	2.68	1.62	1.59
2	A	701	ANP	C8-N9	-2.59	1.33	1.37
2	D	701	ANP	PG-O3G	-2.54	1.50	1.56
2	A	701	ANP	PG-O2G	-2.52	1.50	1.56
2	B	701	ANP	PA-O1A	-2.51	1.42	1.50
2	C	701	ANP	PA-O1A	-2.46	1.42	1.50
2	B	701	ANP	C6-N1	-2.38	1.29	1.35
2	D	701	ANP	C4-N9	-2.38	1.32	1.37
2	B	701	ANP	PB-N3B	2.29	1.69	1.63
2	D	701	ANP	C6-N6	2.26	1.40	1.34
2	D	701	ANP	C5-C4	-2.13	1.35	1.39
2	D	701	ANP	C6-N1	-2.09	1.29	1.35
2	C	701	ANP	C6-N1	-2.03	1.30	1.35

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	-8.41	91.83	109.87
2	B	701	ANP	C5-C4-N3	-7.06	116.99	126.72
2	B	701	ANP	O3G-PG-O1G	-6.95	96.03	113.45
2	B	701	ANP	N3-C2-N1	-6.52	118.72	128.58
2	D	701	ANP	N3-C2-N1	-6.00	119.50	128.58
2	B	701	ANP	C4-C5-N7	-5.81	103.94	110.58
2	C	701	ANP	N3-C2-N1	-5.69	119.97	128.58
2	D	701	ANP	C5-C4-N3	-5.51	119.12	126.72
2	C	701	ANP	C5-C4-N3	-5.51	119.13	126.72
2	B	701	ANP	C2-N3-C4	5.37	124.94	111.83
2	D	701	ANP	O3A-PB-N3B	5.32	121.35	106.59
2	A	701	ANP	N3-C2-N1	-5.24	120.64	128.58
2	A	701	ANP	C3'-C2'-C1'	5.00	110.92	101.46
2	A	701	ANP	C5-C4-N3	-4.81	120.09	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	ANP	O2G-PG-O1G	-4.76	101.52	113.45
2	C	701	ANP	C2-N3-C4	4.58	123.01	111.83
2	D	701	ANP	C2-N3-C4	4.48	122.76	111.83
2	B	701	ANP	C5-C4-N9	4.41	110.62	105.81
2	D	701	ANP	C4-C5-N7	-4.12	105.87	110.58
2	C	701	ANP	O2G-PG-O3G	4.01	118.37	107.59
2	C	701	ANP	O1G-PG-N3B	-3.94	105.97	111.77
2	A	701	ANP	C2-N3-C4	3.82	121.17	111.83
2	B	701	ANP	C5-N7-C8	3.57	109.05	103.45
2	D	701	ANP	O2B-PB-O1B	3.55	117.49	109.87
2	A	701	ANP	C2'-C3'-C4'	-3.47	95.90	102.61
2	C	701	ANP	C3'-C2'-C1'	3.36	107.81	101.46
2	A	701	ANP	C4-C5-N7	-3.28	106.83	110.58
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
2	C	701	ANP	C4-C5-N7	-3.25	106.87	110.58
2	B	701	ANP	N3-C4-N9	3.07	132.39	127.17
2	B	701	ANP	C6-C5-N7	3.02	137.92	132.09
2	D	701	ANP	C5-N7-C8	3.02	108.19	103.45
2	C	701	ANP	C5-C4-N9	3.01	109.09	105.81
2	D	701	ANP	N3-C4-N9	2.96	132.21	127.17
2	D	701	ANP	O2B-PB-O3A	2.85	114.15	104.64
2	A	701	ANP	O4'-C4'-C3'	2.82	110.75	105.15
2	D	701	ANP	C2-N1-C6	2.76	123.26	118.73
2	A	701	ANP	N3-C4-N9	2.73	131.81	127.17
2	C	701	ANP	N3-C4-N9	2.71	131.78	127.17
2	A	701	ANP	N9-C8-N7	-2.69	110.12	113.94
2	D	701	ANP	C5-C4-N9	2.62	108.67	105.81
2	B	701	ANP	C2-N1-C6	2.62	123.03	118.73
2	C	701	ANP	O2B-PB-O1B	2.57	115.38	109.87
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	D	701	ANP	C3'-C2'-C1'	2.48	106.15	101.46
2	D	701	ANP	C6-C5-N7	2.46	136.84	132.09
2	C	701	ANP	C2-N1-C6	2.46	122.76	118.73
2	A	701	ANP	C5-N7-C8	2.41	107.24	103.45
2	B	701	ANP	O3A-PB-N3B	2.38	113.20	106.59
2	C	701	ANP	C2'-C3'-C4'	-2.29	98.17	102.61
2	C	701	ANP	C5-N7-C8	2.19	106.89	103.45
2	A	701	ANP	C6-C5-N7	2.14	136.22	132.09
2	D	701	ANP	O2G-PG-O1G	-2.10	108.19	113.45
2	A	701	ANP	C5-C4-N9	2.09	108.09	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	ANP	C6-C5-N7	2.09	136.12	132.09
2	B	701	ANP	O2G-PG-O3G	-2.05	102.07	107.59
2	D	701	ANP	O2G-PG-O3G	2.05	113.10	107.59

There are no chirality outliers.

All (59) 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	A	701	ANP	C5'-O5'-PA-O3A
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	B	701	ANP	C5'-O5'-PA-O3A
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	C	701	ANP	C5'-O5'-PA-O3A
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
2	D	701	ANP	C5'-O5'-PA-O3A
3	A	702	MYR	C1-C2-C3-C4
3	D	702	MYR	C10-C11-C12-C13
3	A	702	MYR	C7-C8-C9-C10
3	C	702	MYR	C3-C4-C5-C6
3	C	702	MYR	C10-C11-C12-C13
3	A	702	MYR	C11-C10-C9-C8
3	B	702	MYR	C3-C4-C5-C6
3	A	702	MYR	C2-C3-C4-C5
3	D	702	MYR	C6-C7-C8-C9
3	B	702	MYR	C7-C8-C9-C10
3	D	702	MYR	C11-C10-C9-C8
3	C	702	MYR	C11-C10-C9-C8
3	C	702	MYR	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	702	MYR	C11-C10-C9-C8
3	D	702	MYR	C3-C4-C5-C6
3	B	702	MYR	C10-C11-C12-C13
3	A	702	MYR	C10-C11-C12-C13
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
2	A	701	ANP	PB-O3A-PA-O5'
2	C	701	ANP	PB-O3A-PA-O5'
3	D	702	MYR	C4-C5-C6-C7
3	D	702	MYR	C2-C3-C4-C5
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	PB-O3A-PA-O1A
2	B	701	ANP	PB-O3A-PA-O1A
2	C	701	ANP	PB-O3A-PA-O1A
2	D	701	ANP	PB-O3A-PA-O1A

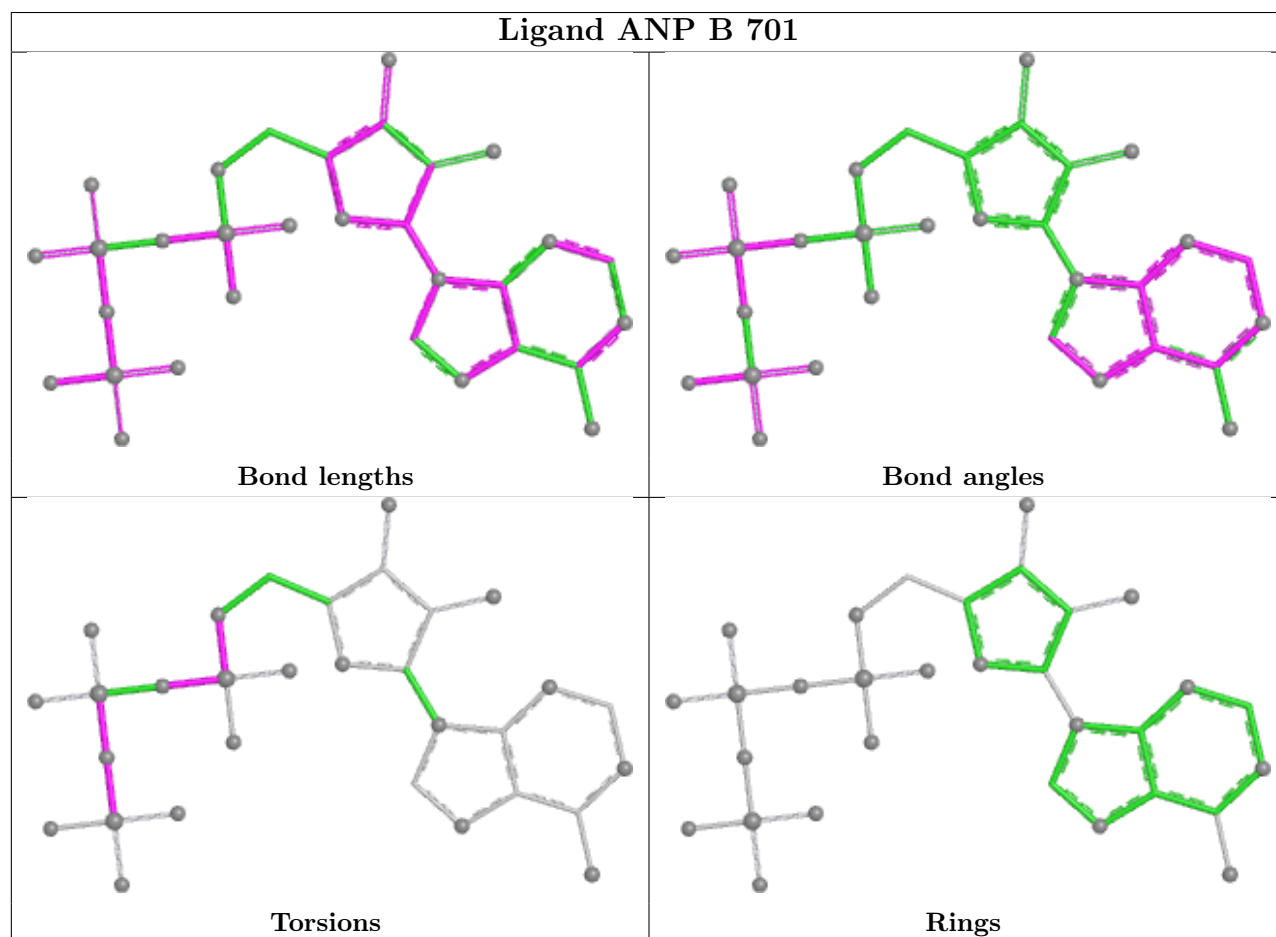
There are no ring outliers.

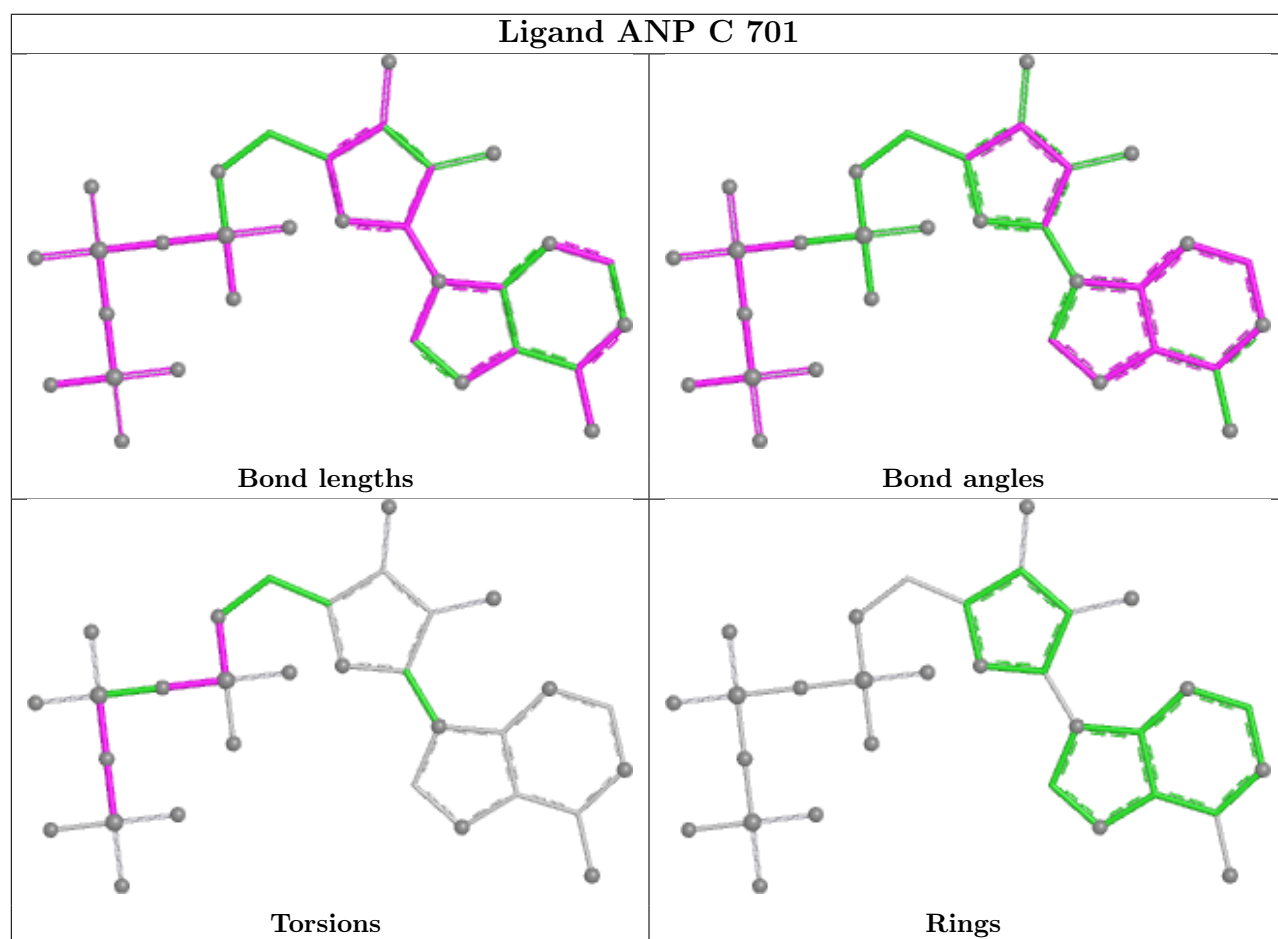
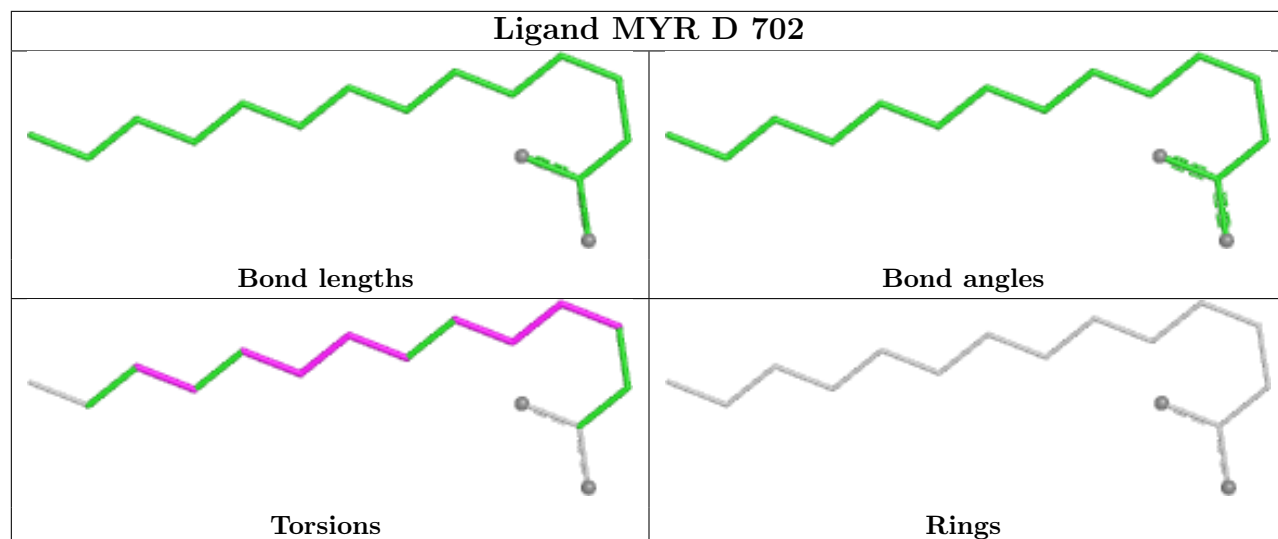
8 monomers are involved in 11 short contacts:

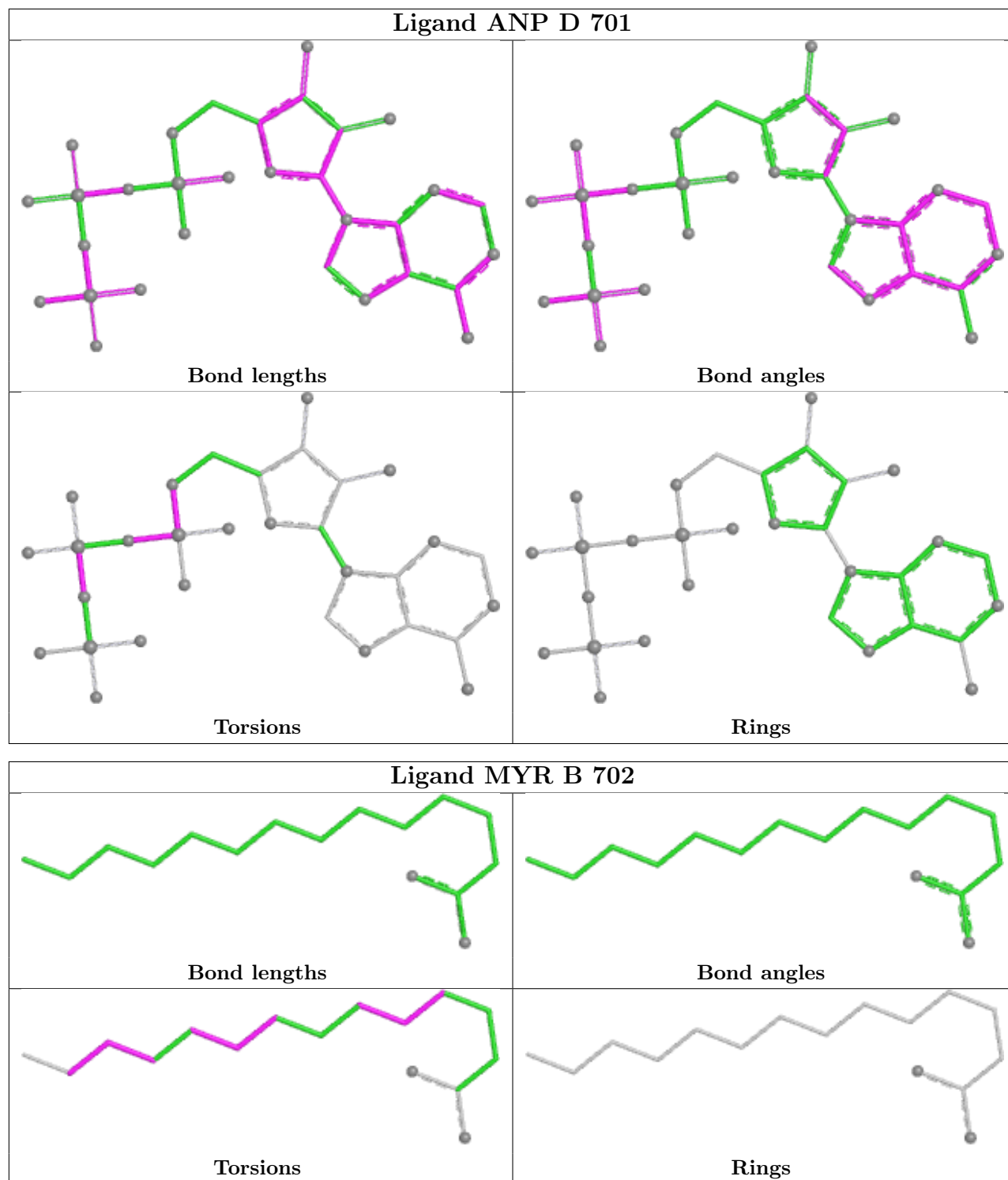
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ANP	1	0
3	D	702	MYR	1	0
2	C	701	ANP	3	0
2	D	701	ANP	1	0
3	B	702	MYR	1	0
3	A	702	MYR	1	0
2	A	701	ANP	1	0
3	C	702	MYR	5	0

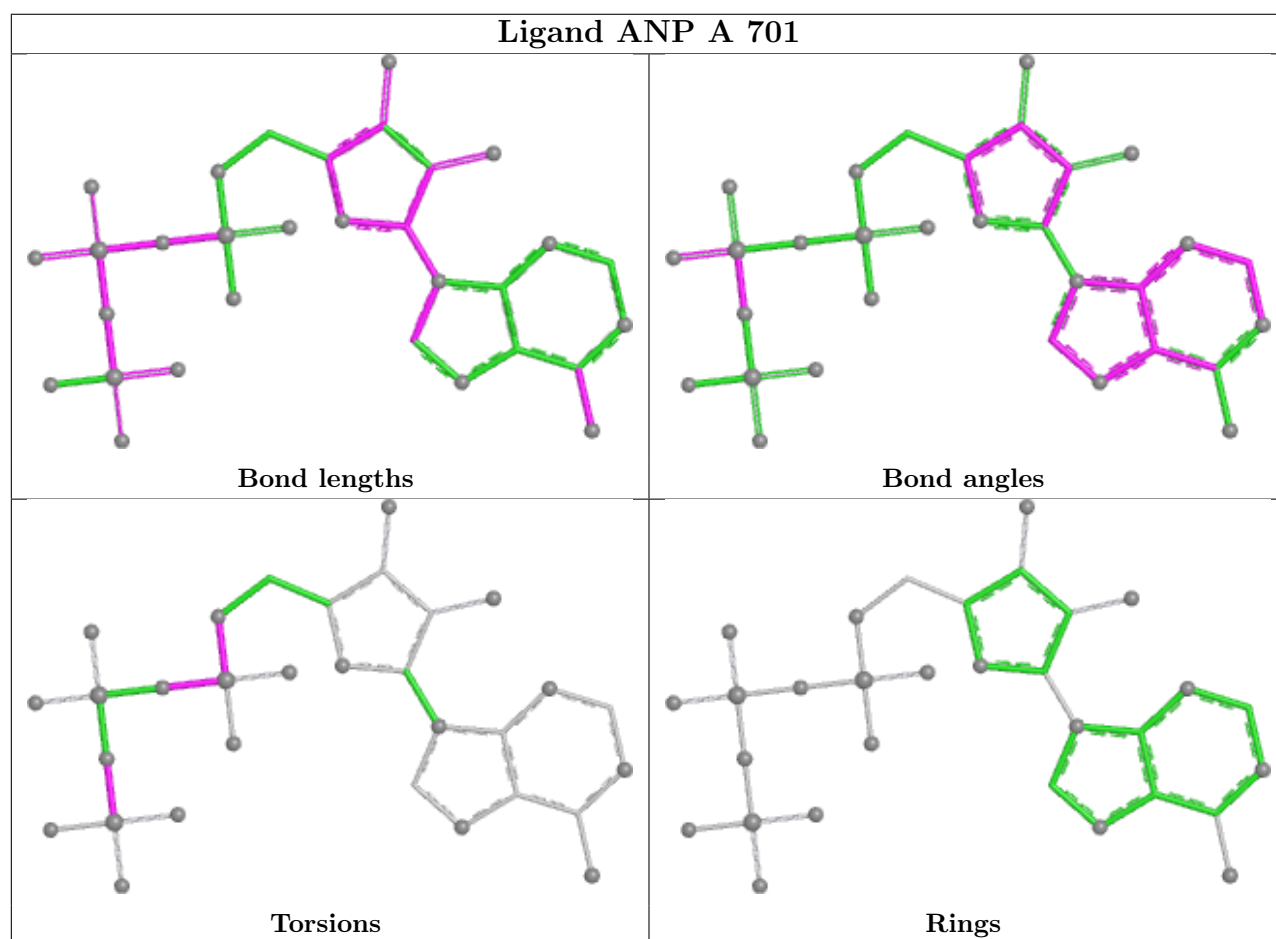
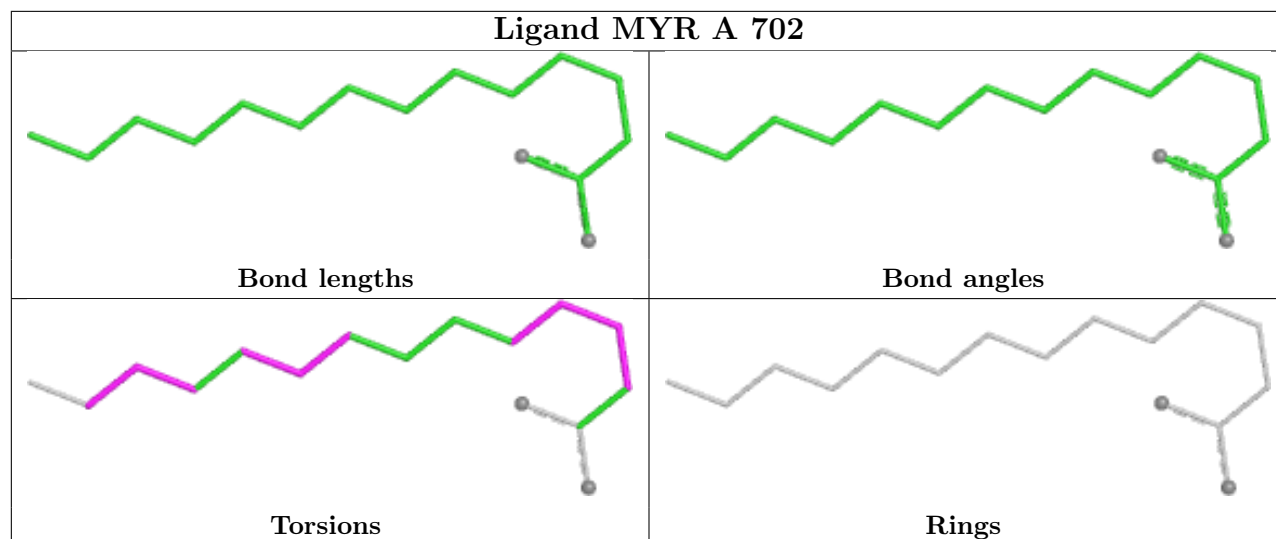
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

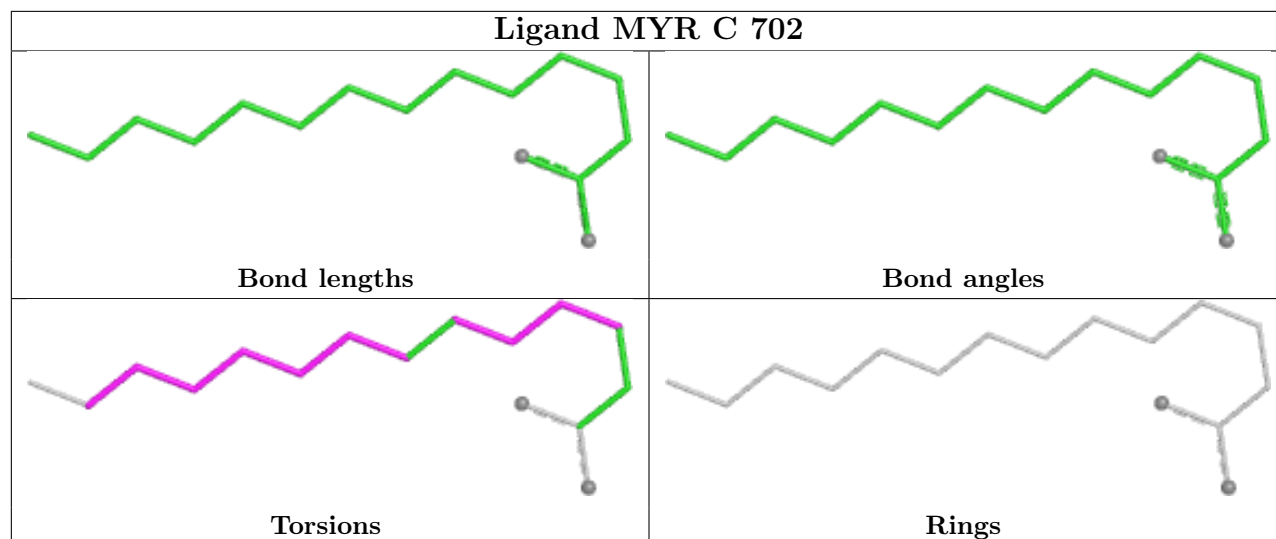
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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	603/604 (99%)	0.10	27 (4%) 38 37	10, 22, 44, 69	0
1	B	597/604 (98%)	0.46	51 (8%) 16 15	11, 29, 54, 80	0
1	C	593/604 (98%)	0.50	68 (11%) 9 8	10, 26, 55, 75	0
1	D	490/604 (81%)	0.12	22 (4%) 38 37	11, 22, 47, 65	0
All	All	2283/2416 (94%)	0.30	168 (7%) 20 19	10, 25, 51, 80	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	589	GLY	11.1
1	C	588	SER	10.4
1	A	534	ALA	10.3
1	A	184	ALA	9.2
1	A	186	ALA	8.6
1	C	584	LEU	7.9
1	A	535	VAL	7.9
1	D	496	LEU	7.8
1	C	595	VAL	7.5
1	A	533	ASP	7.3
1	C	591	ILE	6.3
1	C	585	ARG	5.6
1	C	579	ALA	5.5
1	C	586	SER	5.4
1	C	582	GLU	5.4
1	B	122	ALA	5.2
1	C	599	ALA	5.1
1	C	598	LYS	5.0
1	A	185	ALA	5.0
1	A	532	GLY	4.8
1	C	587	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	583	ILE	4.7
1	C	37	VAL	4.6
1	C	546	LEU	4.6
1	C	522	PRO	4.6
1	D	285	GLY	4.5
1	C	580	PRO	4.5
1	C	120	GLY	4.4
1	A	13	ALA	4.4
1	C	3	LEU	4.4
1	C	590	LYS	4.3
1	C	596	ASN	4.3
1	B	120	GLY	4.0
1	C	182	SER	3.9
1	C	524	ALA	3.9
1	B	392	ASP	3.8
1	C	592	ALA	3.8
1	B	178	ILE	3.8
1	D	495	ASP	3.7
1	C	594	ARG	3.7
1	B	460	ASN	3.6
1	C	54	GLY	3.6
1	A	392	ASP	3.6
1	C	200	THR	3.5
1	B	202	GLY	3.5
1	C	525	VAL	3.5
1	C	520	ILE	3.4
1	C	593	ARG	3.4
1	D	391	GLY	3.4
1	B	530	ILE	3.4
1	C	528	PHE	3.4
1	D	13	ALA	3.4
1	C	515	HIS	3.3
1	C	119	PRO	3.3
1	D	309	GLU	3.3
1	B	6	ALA	3.3
1	D	14	LYS	3.2
1	A	284	GLU	3.2
1	C	523	ALA	3.2
1	C	511	TYR	3.1
1	B	391	GLY	3.1
1	A	187	ALA	3.1
1	A	15	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	4	HIS	3.1
1	A	37	VAL	3.0
1	A	604	HIS	3.0
1	B	204	THR	3.0
1	A	201	SER	3.0
1	D	119	PRO	3.0
1	D	181	PRO	3.0
1	C	578	VAL	2.9
1	A	391	GLY	2.9
1	B	285	GLY	2.9
1	D	200	THR	2.9
1	B	539	ILE	2.9
1	D	4	HIS	2.8
1	B	551	SER	2.8
1	C	597	LYS	2.8
1	A	203	SER	2.8
1	C	484	ASP	2.8
1	C	5	LYS	2.8
1	B	200	THR	2.8
1	D	460	ASN	2.7
1	A	14	LYS	2.7
1	C	531	GLU	2.7
1	C	539	ILE	2.7
1	B	573	ALA	2.7
1	C	13	ALA	2.7
1	B	272	GLN	2.7
1	B	181	PRO	2.7
1	C	499	ILE	2.7
1	B	531	GLU	2.6
1	C	121	HIS	2.6
1	A	8	GLY	2.6
1	C	581	ASP	2.6
1	A	306	THR	2.6
1	C	183	MET	2.6
1	C	118	GLU	2.6
1	B	310	GLY	2.6
1	B	562	ALA	2.6
1	B	571	VAL	2.6
1	C	534	ALA	2.6
1	C	158	GLN	2.5
1	C	541	LEU	2.5
1	D	393	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	56	VAL	2.5
1	B	499	ILE	2.5
1	B	565	THR	2.5
1	C	507	GLN	2.5
1	B	306	THR	2.5
1	C	206	THR	2.5
1	D	52	THR	2.4
1	C	393	ASN	2.4
1	B	309	GLU	2.4
1	B	394	ALA	2.4
1	D	122	ALA	2.4
1	C	576	ARG	2.4
1	C	122	ALA	2.4
1	A	285	GLY	2.4
1	A	5	LYS	2.4
1	B	5	LYS	2.4
1	B	498	ILE	2.3
1	A	460	ASN	2.3
1	D	37	VAL	2.3
1	C	512	THR	2.3
1	B	201	SER	2.3
1	B	500	ALA	2.3
1	A	120	GLY	2.3
1	D	8	GLY	2.3
1	C	543	GLU	2.3
1	C	535	VAL	2.3
1	B	527	ALA	2.2
1	B	529	ALA	2.2
1	B	602	GLU	2.2
1	B	203	SER	2.2
1	C	547	ASP	2.2
1	C	444	GLU	2.2
1	D	118	GLU	2.2
1	D	206	THR	2.2
1	B	537	GLN	2.2
1	D	3	LEU	2.2
1	D	158	GLN	2.2
1	B	308	SER	2.2
1	B	179	PRO	2.2
1	C	303	ARG	2.2
1	C	392	ASP	2.2
1	B	119	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	529	ALA	2.2
1	B	566	GLU	2.1
1	C	532	GLY	2.1
1	B	233	PRO	2.1
1	A	53	GLU	2.1
1	B	123	ASP	2.1
1	B	547	ASP	2.1
1	C	514	ASP	2.1
1	A	202	GLY	2.1
1	B	564	VAL	2.1
1	B	569	GLY	2.1
1	B	554	ALA	2.1
1	C	117	SER	2.0
1	B	501	GLY	2.0
1	B	177	GLN	2.0
1	C	513	VAL	2.0
1	B	41	ASP	2.0
1	C	533	ASP	2.0
1	D	392	ASP	2.0
1	A	308	SER	2.0
1	B	393	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

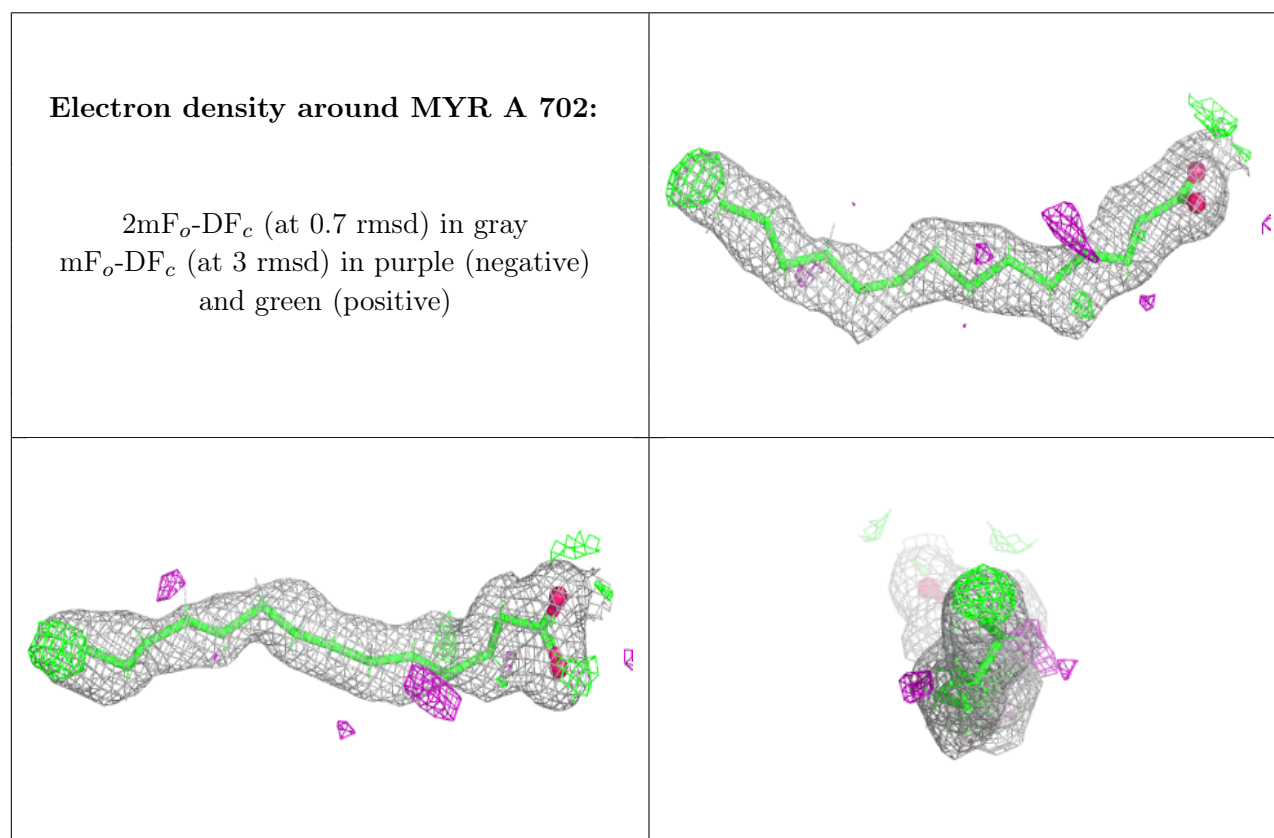
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	703	1/1	0.64	0.14	30,30,30,30	0
4	MG	A	703	1/1	0.65	0.14	30,30,30,30	0

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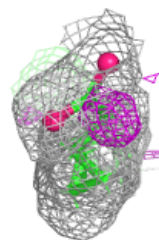
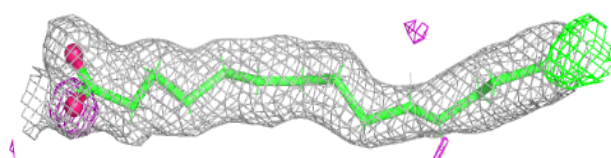
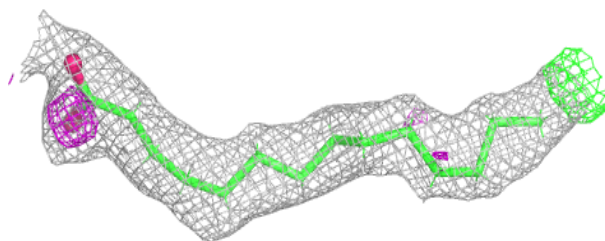
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MYR	A	702	16/16	0.87	0.13	19,37,48,50	0
3	MYR	D	702	16/16	0.90	0.09	21,31,44,46	0
3	MYR	B	702	16/16	0.91	0.09	20,35,49,55	0
3	MYR	C	702	16/16	0.92	0.10	25,35,46,50	0
2	ANP	C	701	31/31	0.93	0.10	17,26,70,93	0
2	ANP	D	701	31/31	0.93	0.09	16,23,66,101	0
2	ANP	B	701	31/31	0.94	0.08	12,21,47,66	0
2	ANP	A	701	31/31	0.97	0.06	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.

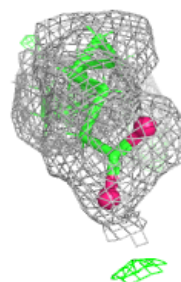
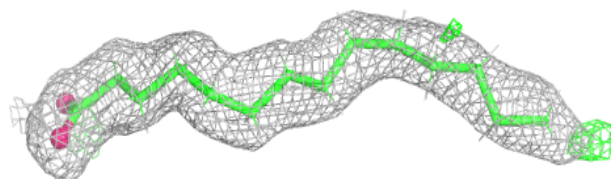
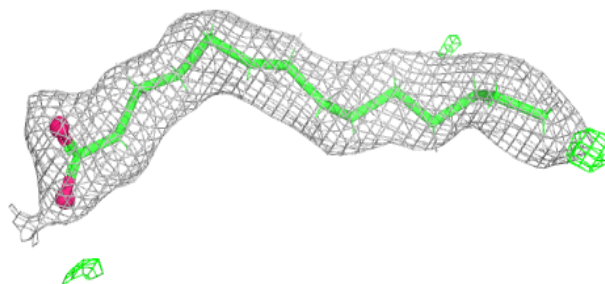


Electron density around MYR D 702:

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

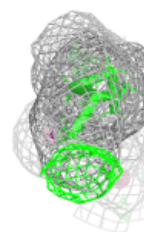
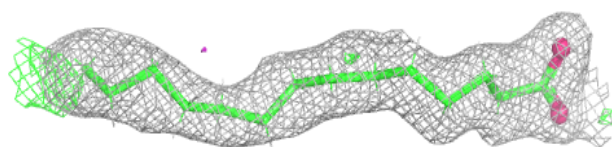
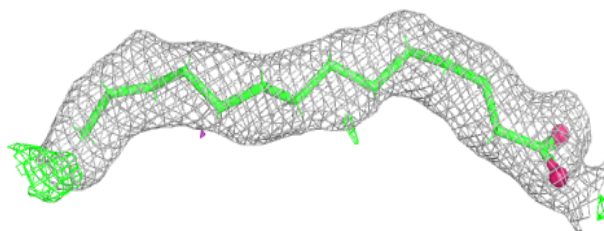
**Electron density around MYR B 702:**

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

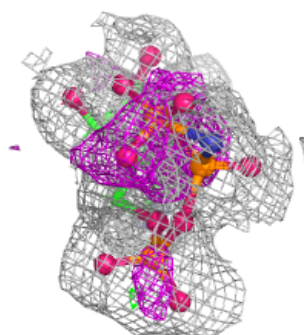
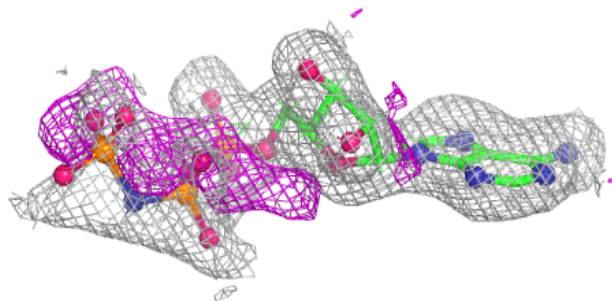
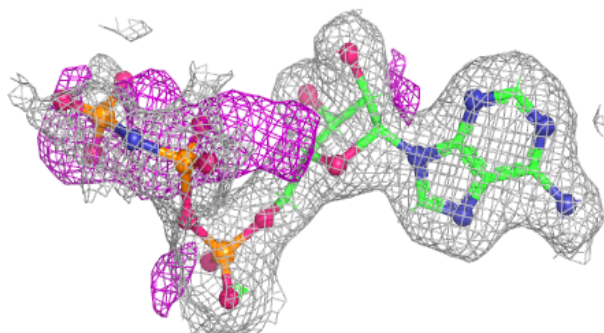


Electron density around MYR C 702:

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

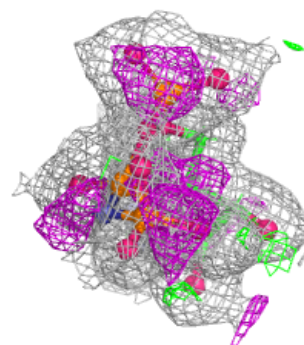
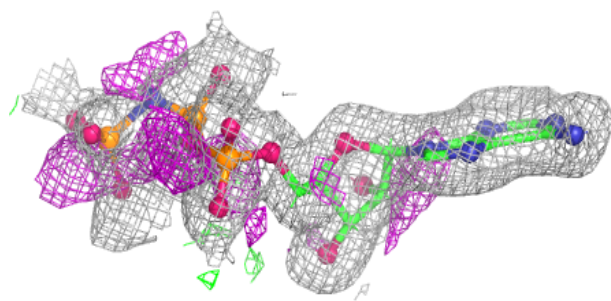
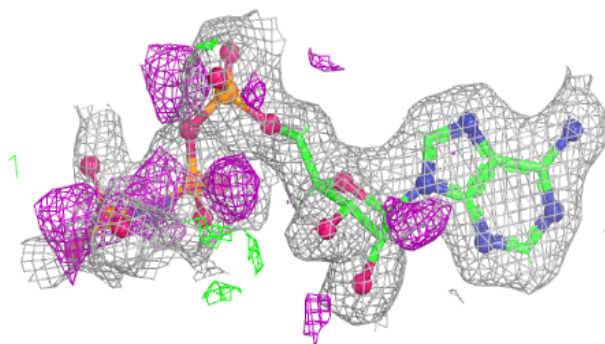
**Electron density around ANP C 701:**

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

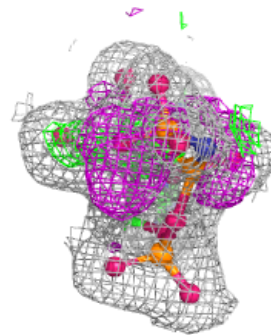
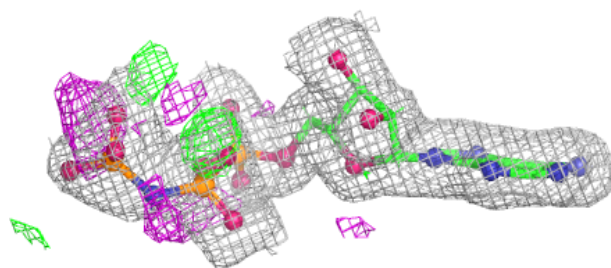
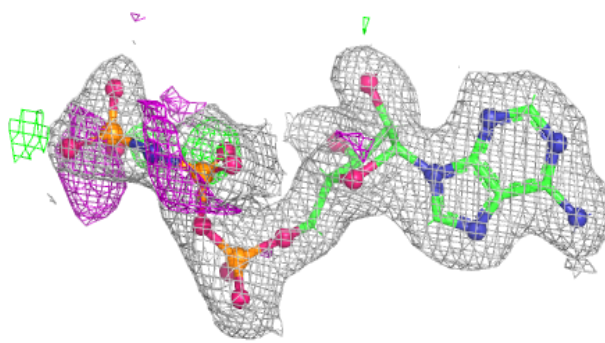


Electron density around ANP D 701:

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

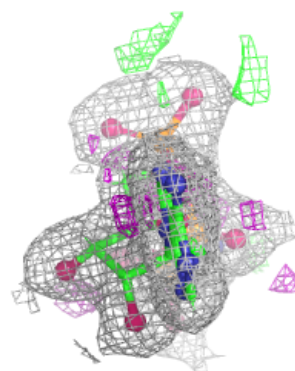
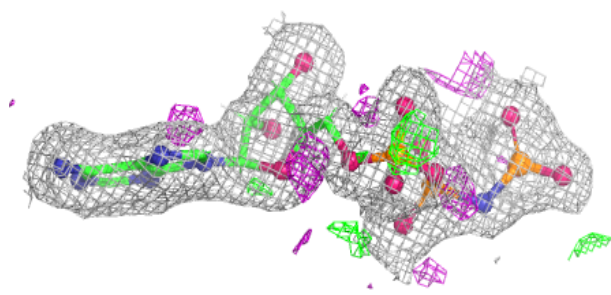
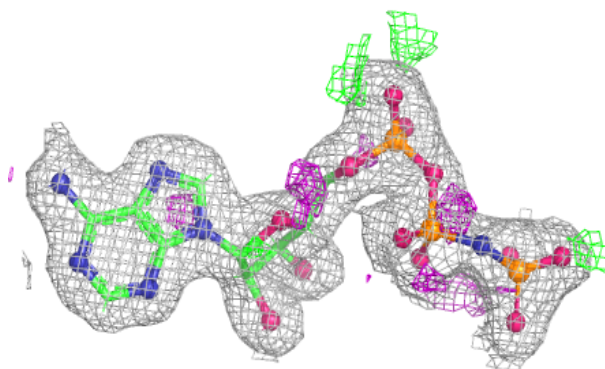
**Electron density around ANP B 701:**

$2mF_o-DF_c$ (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.