



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:04 am BST

PDB ID : 5YJX
Title : Structure of the Ndi1 protein from *Saccharomyces cerevisiae* in complex with myxothiazol.
Authors : Yamasita, T.; Inaoka, D.K.; Shiba, T.; Oohashi, T.; Iwata, S.; Yagi, T.; Kosaka, H.; Harada, S.; Kita, K.; Hirano, K.
Deposited on : 2017-10-11
Resolution : 3.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

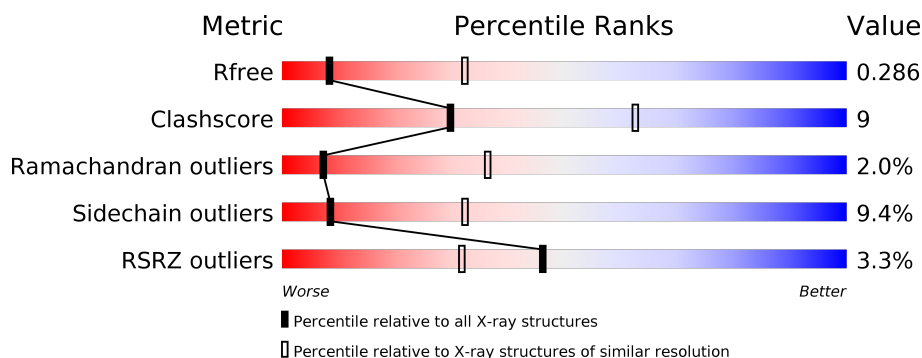
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>• 5%</div> </div> </div>
1	B	486	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MYX	B	607	-	-	-	X

2 Entry composition ⓘ

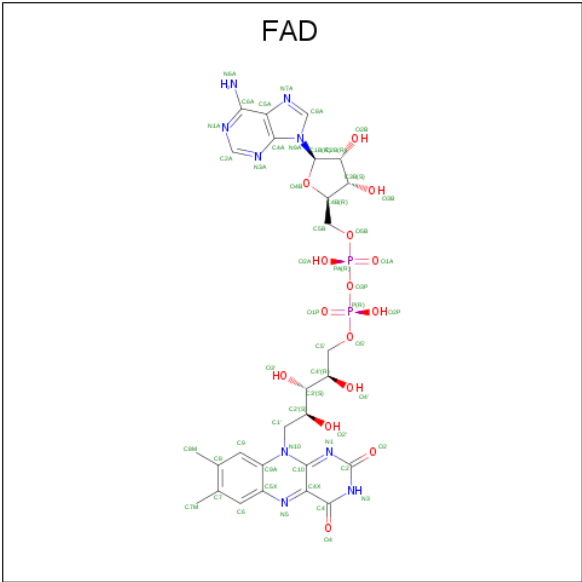
There are 5 unique types of molecules in this entry. The entry contains 7563 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	3	0
			3673	2373	620	675	5			
1	B	464	Total	C	N	O	S	0	4	0
			3686	2381	623	677	5			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by author).

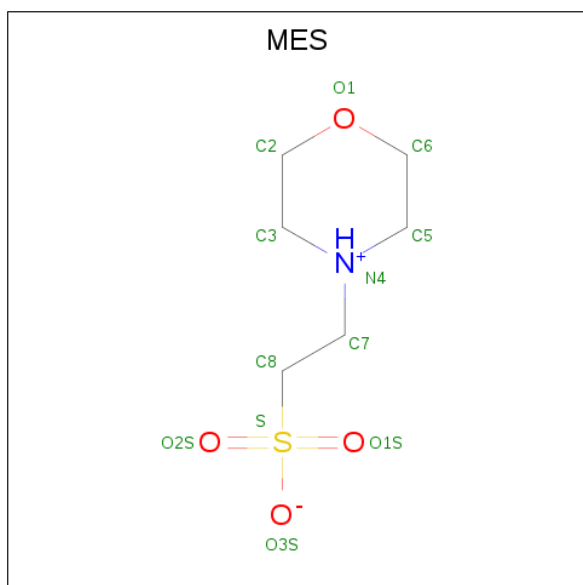


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

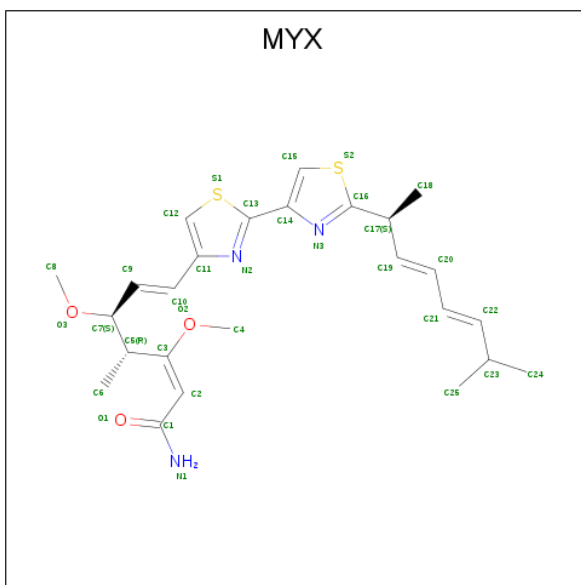
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Mg 4 4	0	0
3	A	4	Total Mg 4 4	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 1 4 1	0	0
4	B	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 5 is (2Z,6E)-7-{2'-[(2E,4E)-1,6-DIMETHYLHEPTA-2,4-DIENYL]-2,4'-BI-1,3-THIAZOL-4-YL}-3,5-DIMETHOXY-4-METHYLHEPTA-2,6-DIENAMIDE (three-letter code: MYX) (formula: C₂₅H₃₃N₃O₃S₂).

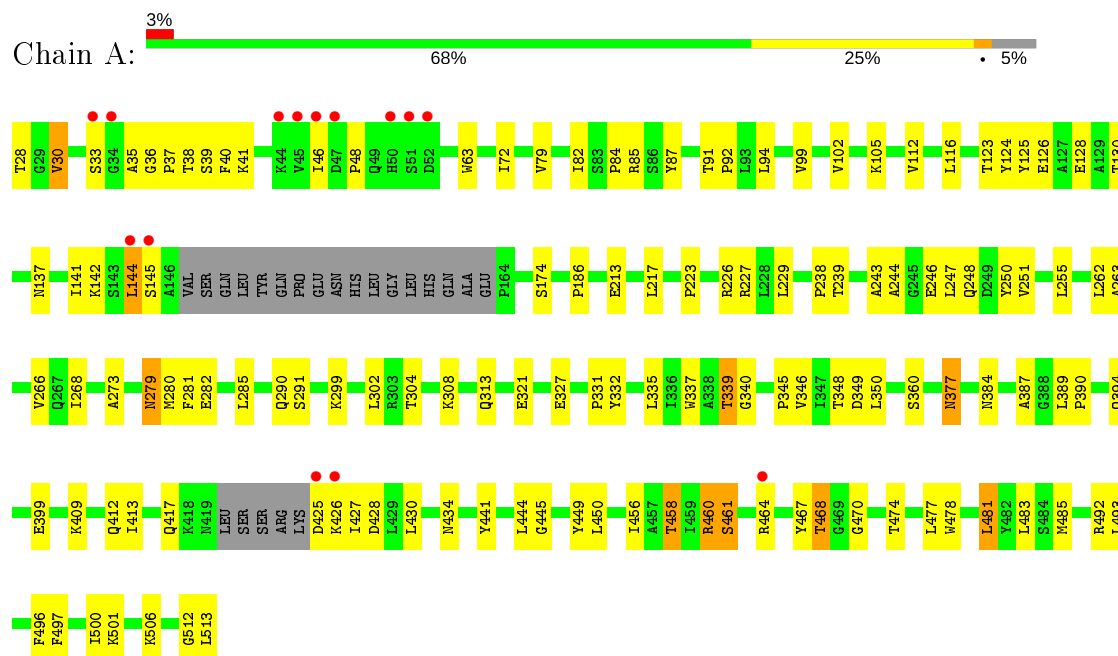


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 33	C 25	N 3	O 3	S 2	0	0
5	B	1	Total 33	C 25	N 3	O 3	S 2	0	0

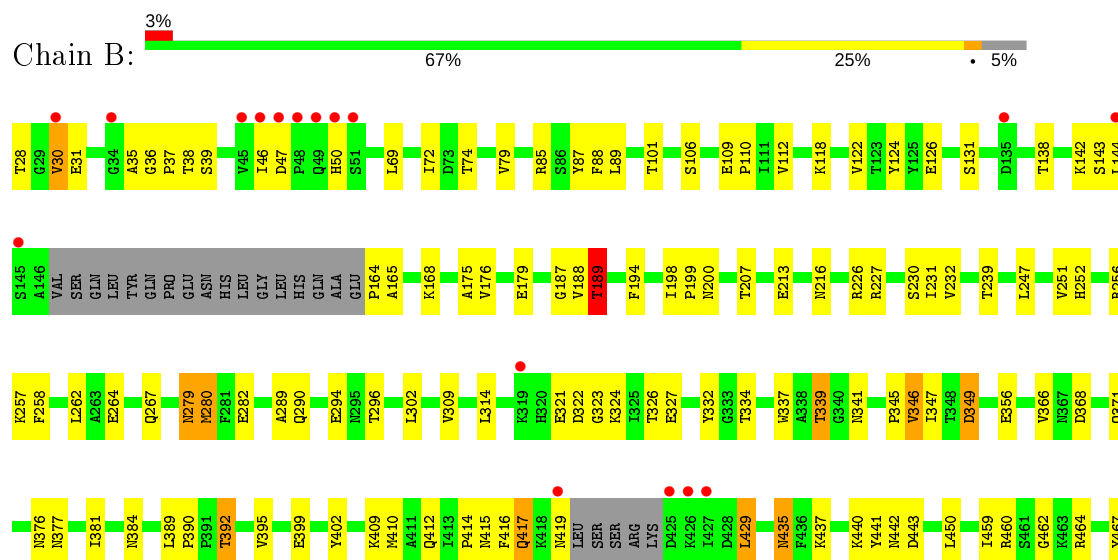
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial



- Molecule 1: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.34Å 116.40Å 166.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.21 19.97 – 3.21	Depositor EDS
% Data completeness (in resolution range)	88.9 (20.00-3.21) 89.2 (19.97-3.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.220 , 0.285 0.224 , 0.286	Depositor DCC
R_{free} test set	1043 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7563	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9395e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MYX, MG, MES, FAD

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	0.41	0/3759	0.61	0/5084
1	B	0.42	0/3768	0.66	1/5096 (0.0%)
All	All	0.41	0/7527	0.63	1/10180 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	189	THR	CB-CA-C	-8.59	88.40	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	417	GLN	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3673	0	3735	79	0
1	B	3686	0	3748	71	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	12	0	13	0	0
4	B	12	0	13	0	0
5	A	33	0	33	5	0
5	B	33	0	33	1	0
All	All	7563	0	7637	143	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 (143) 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:A:450:LEU:HD11	1:A:456:ILE:HG23	1.61	0.81
1:B:36:GLY:HA3	1:B:126:GLU:O	1.81	0.80
1:A:493:LEU:HD11	1:A:497:PHE:CZ	2.17	0.80
1:B:232:VAL:HG11	1:B:314:LEU:HD21	1.72	0.71
1:A:512:GLY:O	1:A:513:LEU:HD12	1.93	0.69
1:A:116:LEU:HD21	1:B:258:PHE:HB3	1.73	0.68
1:B:230:SER:OG	1:B:332:TYR:HA	1.94	0.68
1:A:460:ARG:HG2	1:A:461:SER:N	2.09	0.67
1:B:390:PRO:HB2	1:B:392:THR:HG23	1.80	0.64
1:B:290:GLN:HE22	1:B:302:LEU:HD11	1.63	0.64
1:A:394:GLN:HA	5:A:607:MYX:H61	1.80	0.64
1:A:30:VAL:O	1:A:30:VAL:HG12	1.98	0.63
1:A:251:VAL:HG21	1:A:266:VAL:HG11	1.81	0.62
1:A:141:ILE:HG13	1:A:141:ILE:O	1.99	0.62
1:A:37:PRO:HB3	1:B:213:GLU:HB3	1.82	0.61
1:A:213:GLU:HB3	1:B:37:PRO:CB	2.30	0.61
1:A:213:GLU:HB3	1:B:37:PRO:HB2	1.82	0.61
1:B:477:LEU:O	1:B:481:LEU:N	2.30	0.61
1:A:493:LEU:HD11	1:A:497:PHE:CE2	2.36	0.60
1:A:290:GLN:NE2	1:A:302:LEU:HD11	2.17	0.60
1:A:445:GLY:HA2	1:A:460:ARG:NH1	2.17	0.59
1:A:458:THR:HG22	1:A:460:ARG:HH12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ASP:OD1	1:B:460:ARG:NH1	2.36	0.59
1:A:82:ILE:HD13	1:A:141:ILE:HG21	1.84	0.59
1:B:496:PHE:CE2	1:B:500:ILE:HD11	2.39	0.58
1:A:82:ILE:HD13	1:A:141:ILE:CG2	2.34	0.58
1:B:493:LEU:HD11	1:B:497:PHE:CE2	2.39	0.57
1:B:486:ILE:O	1:B:492:ARG:NH2	2.36	0.57
1:A:63:TRP:CH2	5:A:607:MYX:H81	2.39	0.57
1:B:74:THR:HG21	1:B:118:LYS:HB3	1.85	0.57
1:B:279:ASN:HD22	1:B:279:ASN:C	2.07	0.56
1:A:279:ASN:HD22	1:A:280:MET:N	2.03	0.56
1:A:255:LEU:HD23	1:A:263:ALA:HA	1.86	0.56
1:A:345:PRO:HA	1:A:348:THR:OG1	2.05	0.56
1:A:229:LEU:HD11	1:A:262:LEU:HD22	1.87	0.55
1:B:390:PRO:HB2	1:B:392:THR:CG2	2.37	0.55
1:A:40:PHE:CE2	1:A:124:TYR:HB3	2.41	0.55
1:B:290:GLN:NE2	1:B:302:LEU:HD11	2.21	0.55
1:A:94:LEU:HB3	2:A:601:FAD:HM72	1.89	0.54
1:B:164:PRO:HB3	1:B:165:ALA:HA	1.88	0.54
1:A:35:ALA:HB2	1:A:141:ILE:CD1	2.37	0.54
1:A:40:PHE:CD1	1:A:40:PHE:C	2.81	0.54
1:B:389:LEU:HD22	1:B:441:TYR:CD2	2.42	0.54
1:B:239:THR:HG23	2:B:601:FAD:HM73	1.89	0.54
1:A:389:LEU:HB3	1:A:390:PRO:HD2	1.91	0.53
1:A:350:LEU:O	1:A:350:LEU:HG	2.09	0.53
1:B:322:ASP:O	1:B:324:LYS:N	2.42	0.52
1:A:37:PRO:O	1:A:39:SER:N	2.36	0.52
1:A:99:VAL:HG21	1:A:246:GLU:O	2.10	0.52
1:A:458:THR:O	1:A:458:THR:HG22	2.10	0.52
1:B:164:PRO:CB	1:B:165:ALA:HA	2.40	0.52
1:B:289:ALA:HA	1:B:450:LEU:HD13	1.92	0.52
1:B:35:ALA:O	1:B:143:SER:CB	2.58	0.52
1:B:227:ARG:NH1	1:B:332:TYR:O	2.43	0.51
1:A:394:GLN:HA	5:A:607:MYX:C6	2.41	0.51
1:B:231:ILE:N	1:B:267:GLN:O	2.37	0.51
1:A:105:LYS:HG2	1:B:513:LEU:HD23	1.93	0.51
1:A:35:ALA:CB	1:A:125:TYR:HB3	2.41	0.50
1:A:84:PRO:HG3	1:A:128:GLU:HB3	1.91	0.50
1:A:217:LEU:HD23	1:A:217:LEU:N	2.27	0.50
1:A:238:PRO:HG2	5:A:607:MYX:C18	2.42	0.50
1:B:459:ILE:HD12	1:B:467:TYR:HB3	1.94	0.50
1:B:230:SER:HG	1:B:332:TYR:HA	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASN:HD22	1:A:279:ASN:C	2.16	0.49
1:A:130:THR:HG21	1:A:142:LYS:HB2	1.95	0.49
1:A:105:LYS:HE3	1:B:513:LEU:HB3	1.95	0.49
1:B:194:PHE:O	1:B:200:ASN:HB3	2.13	0.48
1:B:252:HIS:O	1:B:256:ARG:HG2	2.13	0.48
1:B:346:VAL:HG23	1:B:347:ILE:HG12	1.94	0.48
1:B:437[B]:LYS:HE2	1:B:437[B]:LYS:N	2.28	0.48
1:A:496:PHE:CE2	1:A:500:ILE:HD11	2.49	0.47
1:B:410:MET:HG2	1:B:416:PHE:CE2	2.49	0.47
1:B:345:PRO:O	1:B:349:ASP:HB3	2.15	0.47
1:A:174:SER:C	1:A:384:ASN:HD21	2.18	0.47
1:B:247:LEU:O	1:B:251:VAL:HG23	2.15	0.47
1:A:229:LEU:HB3	1:A:266:VAL:HA	1.97	0.47
1:B:442:ASN:HD21	1:B:462:GLY:H	1.63	0.47
1:B:35:ALA:O	1:B:143:SER:HB3	2.15	0.46
1:A:313:GLN:HA	1:A:331:PRO:HA	1.97	0.46
1:B:395:VAL:O	1:B:399:GLU:HG3	2.16	0.46
1:B:138:THR:HG22	1:B:168:LYS:HA	1.98	0.46
1:A:281:PHE:CE2	1:A:456:ILE:HG13	2.50	0.46
1:B:207:THR:HG21	1:B:334:THR:HG23	1.98	0.46
1:B:314:LEU:O	1:B:314:LEU:HD12	2.15	0.46
1:B:429[A]:LEU:HD23	1:B:429[A]:LEU:N	2.30	0.46
1:B:175:ALA:HB2	1:B:381:ILE:HG13	1.97	0.46
1:B:216:ASN:HB2	1:B:262:LEU:HD11	1.98	0.45
1:B:187:GLY:HA3	1:B:309:VAL:O	2.15	0.45
1:A:282:GLU:HG3	1:A:285:LEU:HD12	1.98	0.45
1:A:512:GLY:C	1:A:513:LEU:HD12	2.37	0.45
1:A:144:LEU:HD13	1:A:144:LEU:C	2.37	0.45
1:A:387:ALA:O	1:A:389:LEU:HG	2.16	0.45
1:B:467:TYR:CG	1:B:468:THR:N	2.85	0.45
1:A:41:LYS:HG2	1:A:123:THR:OG1	2.17	0.45
1:A:460:ARG:HH11	1:A:460:ARG:HB3	1.82	0.45
1:A:91:THR:N	1:A:92:PRO:CD	2.80	0.44
1:B:290:GLN:OE1	1:B:302:LEU:HD11	2.17	0.44
1:B:38:THR:OG1	1:B:124:TYR:CE2	2.70	0.44
1:A:248:GLN:NE2	1:A:268:ILE:HD12	2.33	0.44
1:A:449:TYR:HB2	1:A:478:TRP:CZ2	2.53	0.44
1:A:279:ASN:ND2	1:A:280:MET:N	2.65	0.44
1:B:356:GLU:OE1	1:B:356:GLU:N	2.51	0.44
1:A:332:TYR:CE2	1:A:335:LEU:HB2	2.53	0.44
1:A:477:LEU:HD12	1:A:481:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TRP:NE1	1:A:339:THR:HG23	2.33	0.43
1:A:483:LEU:CD2	1:A:492:ARG:HG3	2.47	0.43
1:A:213:GLU:HB3	1:B:37:PRO:HB3	1.99	0.43
1:A:485:MET:HE3	5:A:607:MYX:H82	2.01	0.43
1:A:223:PRO:O	1:A:226:ARG:N	2.52	0.43
1:B:188:VAL:C	1:B:189:THR:HG23	2.39	0.43
1:B:341[B]:ASN:N	1:B:341[B]:ASN:OD1	2.51	0.43
1:A:39:SER:HA	1:A:124:TYR:O	2.19	0.42
1:A:186:PRO:HG2	1:A:308:LYS:HB2	2.01	0.42
1:A:85:ARG:HD2	1:A:87:TYR:CE2	2.55	0.42
1:B:85:ARG:HD2	1:B:87:TYR:CE2	2.54	0.42
1:B:142:LYS:CE	1:B:165:ALA:HB3	2.50	0.42
1:A:412:GLN:C	1:A:413:ILE:HG13	2.40	0.42
1:B:176:VAL:HG22	1:B:384:ASN:ND2	2.35	0.42
1:B:30:VAL:HG22	1:B:31:GLU:H	1.85	0.42
1:B:198:ILE:N	1:B:199:PRO:HD2	2.35	0.42
1:A:243:ALA:O	1:A:244:ALA:C	2.59	0.42
1:B:87:TYR:HA	1:B:110:PRO:HA	2.02	0.42
1:B:207:THR:CG2	1:B:334:THR:HG23	2.50	0.42
1:B:437[B]:LYS:HA	1:B:437[B]:LYS:HD3	1.84	0.42
1:A:467:TYR:CG	1:A:468:THR:N	2.88	0.41
1:A:273:ALA:HA	1:A:304:THR:O	2.21	0.41
1:A:394:GLN:NE2	1:A:441:TYR:OH	2.54	0.41
1:B:88:PHE:N	1:B:109:GLU:O	2.46	0.41
1:B:279:ASN:HD22	1:B:280:MET:N	2.18	0.41
1:B:337:TRP:NE1	1:B:339:THR:HG23	2.35	0.41
1:B:435:ASN:OD1	1:B:435:ASN:N	2.53	0.41
1:B:392:THR:HG22	5:B:607:MYX:H20	2.02	0.41
1:B:414:PRO:HA	1:B:417:GLN:HG2	2.02	0.41
1:A:377:ASN:HD22	1:A:377:ASN:H	1.69	0.41
1:B:187:GLY:C	1:B:188:VAL:O	2.56	0.41
1:B:69:LEU:CD1	1:B:79:VAL:HG11	2.51	0.41
1:A:37:PRO:C	1:A:39:SER:H	2.22	0.40
1:A:99:VAL:HB	1:A:250:TYR:HB2	2.04	0.40
1:A:247:LEU:O	1:A:250:TYR:N	2.55	0.40
1:A:72:ILE:HG21	1:A:79:VAL:HG21	2.04	0.40
1:A:227:ARG:HG3	1:A:331:PRO:HB2	2.04	0.40
1:A:36:GLY:HA2	1:A:145:SER:O	2.21	0.40
1:A:470:GLY:HA3	1:A:474:THR:OG1	2.21	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	461/486 (95%)	400 (87%)	51 (11%)	10 (2%)	6	34
1	B	462/486 (95%)	386 (84%)	67 (14%)	9 (2%)	8	38
All	All	923/972 (95%)	786 (85%)	118 (13%)	19 (2%)	7	35

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	ARG
1	A	506	LYS
1	B	323	GLY
1	B	429[A]	LEU
1	B	429[B]	LEU
1	A	126	GLU
1	A	340	GLY
1	A	399	GLU
1	B	39	SER
1	B	106	SER
1	B	189	THR
1	A	239	THR
1	A	458	THR
1	A	33	SER
1	A	38	THR
1	B	376	ASN
1	A	30	VAL
1	B	112	VAL
1	B	72	ILE

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	396/413 (96%)	365 (92%)	31 (8%)	12	42
1	B	397/413 (96%)	354 (89%)	43 (11%)	6	26
All	All	793/826 (96%)	719 (91%)	74 (9%)	8	32

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	46	ILE
1	A	48	PRO
1	A	102	VAL
1	A	112	VAL
1	A	137	ASN
1	A	144	LEU
1	A	279	ASN
1	A	291	SER
1	A	299	LYS
1	A	321	GLU
1	A	327	GLU
1	A	339	THR
1	A	346	VAL
1	A	349	ASP
1	A	360	SER
1	A	377	ASN
1	A	409	LYS
1	A	417	GLN
1	A	425	ASP
1	A	426	LYS
1	A	427	ILE
1	A	428	ASP
1	A	430	LEU
1	A	434	ASN
1	A	444	LEU
1	A	460	ARG
1	A	461	SER
1	A	468	THR
1	A	481	LEU
1	A	501	LYS
1	B	28	THR
1	B	30	VAL

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Mol	Chain	Res	Type
1	B	46	ILE
1	B	47	ASP
1	B	50	HIS
1	B	89	LEU
1	B	101	THR
1	B	122	VAL
1	B	131	SER
1	B	144	LEU
1	B	179	GLU
1	B	189	THR
1	B	226	ARG
1	B	257	LYS
1	B	264	GLU
1	B	279	ASN
1	B	280	MET
1	B	282	GLU
1	B	294	GLU
1	B	296	THR
1	B	321	GLU
1	B	326	THR
1	B	327	GLU
1	B	339	THR
1	B	346	VAL
1	B	349	ASP
1	B	366	VAL
1	B	368	ASP
1	B	371	GLN
1	B	377	ASN
1	B	392	THR
1	B	402	TYR
1	B	409	LYS
1	B	412	GLN
1	B	415	ASN
1	B	419	ASN
1	B	435	ASN
1	B	440	LYS
1	B	464	ARG
1	B	468	THR
1	B	474	THR
1	B	501	LYS
1	B	513	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	248	GLN
1	A	279	ASN
1	A	290	GLN
1	A	377	ASN
1	A	394	GLN
1	A	415	ASN
1	A	442	ASN
1	B	32	ASN
1	B	137	ASN
1	B	200	ASN
1	B	248	GLN
1	B	253	GLN
1	B	279	ASN
1	B	377	ASN
1	B	397	HIS
1	B	417	GLN
1	B	442	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MYX	B	607	-	29,34,34	1.41	2 (6%)	21,45,45	1.49	4 (19%)
4	MES	B	606	-	12,12,12	2.09	1 (8%)	14,16,16	1.63	3 (21%)
4	MES	A	606	-	12,12,12	2.22	1 (8%)	14,16,16	1.35	1 (7%)
2	FAD	A	601	3	51,58,58	1.89	7 (13%)	60,89,89	2.13	14 (23%)
2	FAD	B	601	3	51,58,58	2.02	7 (13%)	60,89,89	2.19	13 (21%)
5	MYX	A	607	-	29,34,34	1.49	4 (13%)	21,45,45	1.79	5 (23%)

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
5	MYX	B	607	-	-	8/25/36/36	0/2/2/2
4	MES	B	606	-	-	0/6/14/14	0/1/1/1
4	MES	A	606	-	-	3/6/14/14	0/1/1/1
2	FAD	A	601	3	-	2/30/50/50	0/6/6/6
2	FAD	B	601	3	-	3/30/50/50	0/6/6/6
5	MYX	A	607	-	-	17/25/36/36	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C4X-C10	10.77	1.49	1.38
2	A	601	FAD	C4X-C10	9.86	1.48	1.38
4	A	606	MES	C8-S	-7.31	1.67	1.77
4	B	606	MES	C8-S	-6.75	1.67	1.77
5	B	607	MYX	O2-C3	5.85	1.46	1.35
5	A	607	MYX	O2-C3	5.77	1.46	1.35
2	A	601	FAD	C4-C4X	4.43	1.49	1.41
2	B	601	FAD	C4-C4X	4.39	1.48	1.41
2	B	601	FAD	C9A-C5X	4.26	1.51	1.42
2	A	601	FAD	C9A-C5X	3.61	1.49	1.42
2	A	601	FAD	C8-C7	3.37	1.49	1.40
2	B	601	FAD	C9A-N10	3.27	1.42	1.38
5	B	607	MYX	C13-N2	3.09	1.35	1.31
2	B	601	FAD	C8-C7	3.08	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	607	MYX	C13-N2	2.89	1.35	1.31
5	A	607	MYX	C15-S2	2.74	1.74	1.70
2	B	601	FAD	C2A-N3A	2.27	1.35	1.32
5	A	607	MYX	C12-S1	2.26	1.74	1.70
2	A	601	FAD	C6-C5X	-2.21	1.38	1.41
2	B	601	FAD	C5A-C4A	2.15	1.46	1.40
2	A	601	FAD	C5A-C4A	2.14	1.46	1.40
2	A	601	FAD	C2A-N3A	2.01	1.35	1.32

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4-N3-C2	9.38	123.06	115.14
2	A	601	FAD	C4-N3-C2	8.90	122.66	115.14
2	B	601	FAD	C1'-N10-C9A	6.85	123.68	118.29
2	A	601	FAD	C1'-N10-C9A	5.77	122.84	118.29
2	A	601	FAD	C4X-C4-N3	-4.81	116.85	123.43
5	A	607	MYX	C18-C17-C19	-4.76	104.82	111.23
2	B	601	FAD	C4X-C4-N3	-4.48	117.31	123.43
2	B	601	FAD	C4-C4X-C10	-4.43	117.02	119.95
2	B	601	FAD	N3A-C2A-N1A	-4.31	121.94	128.68
4	B	606	MES	O3S-S-C8	4.20	112.57	105.77
2	A	601	FAD	N3A-C2A-N1A	-4.18	122.14	128.68
2	A	601	FAD	C4X-N5-C5X	4.06	120.83	116.77
4	A	606	MES	O3S-S-C8	3.92	112.10	105.77
5	B	607	MYX	C4-O2-C3	3.79	122.87	116.52
2	A	601	FAD	P-O3P-PA	-3.64	120.35	132.83
2	B	601	FAD	C4X-N5-C5X	3.47	120.24	116.77
2	A	601	FAD	C4-C4X-C10	-3.27	117.79	119.95
2	B	601	FAD	C9A-N10-C10	-3.19	117.73	121.91
2	B	601	FAD	C4-C4X-N5	3.16	122.21	118.60
5	A	607	MYX	C4-O2-C3	3.13	121.76	116.52
2	A	601	FAD	C9A-N10-C10	-3.09	117.86	121.91
2	A	601	FAD	C4-C4X-N5	3.03	122.06	118.60
2	B	601	FAD	C4'-C3'-C2'	-2.99	107.15	113.36
2	A	601	FAD	C4A-C5A-N7A	-2.94	106.33	109.40
4	B	606	MES	O2S-S-C8	2.91	110.42	106.92
5	A	607	MYX	C14-C15-S2	-2.90	108.23	111.79
2	B	601	FAD	C4A-C5A-N7A	-2.88	106.39	109.40
5	B	607	MYX	O3-C7-C5	2.88	113.77	107.87
2	B	601	FAD	P-O3P-PA	-2.71	123.53	132.83
5	B	607	MYX	C14-C15-S2	-2.57	108.63	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C1B-N9A-C4A	-2.50	122.25	126.64
2	A	601	FAD	O4B-C1B-C2B	-2.47	103.32	106.93
2	A	601	FAD	C4'-C3'-C2'	-2.33	108.52	113.36
2	A	601	FAD	O2P-P-O1P	2.32	123.72	112.24
2	B	601	FAD	C2A-N1A-C6A	2.21	122.53	118.75
5	B	607	MYX	C23-C22-C21	-2.13	121.69	126.19
4	B	606	MES	O3S-S-O2S	-2.12	106.10	111.27
2	B	601	FAD	O2P-P-O1P	2.05	122.39	112.24
5	A	607	MYX	C23-C22-C21	-2.05	121.86	126.19
5	A	607	MYX	C2-C1-N1	2.04	122.81	115.61

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	607	MYX	C2-C3-O2-C4
5	B	607	MYX	C5-C3-O2-C4
5	B	607	MYX	C3-C5-C7-C9
5	B	607	MYX	C6-C5-C7-O3
5	B	607	MYX	C6-C5-C7-C9
5	B	607	MYX	O3-C7-C9-C10
4	A	606	MES	C7-C8-S-O1S
4	A	606	MES	C7-C8-S-O3S
2	A	601	FAD	PA-O3P-P-O5'
5	A	607	MYX	C2-C3-O2-C4
5	A	607	MYX	C5-C3-O2-C4
5	A	607	MYX	C2-C3-C5-C7
5	A	607	MYX	C3-C5-C7-C9
5	A	607	MYX	C6-C5-C7-C9
5	A	607	MYX	C5-C7-C9-C10
5	A	607	MYX	O3-C7-C9-C10
5	A	607	MYX	O2-C3-C5-C7
5	A	607	MYX	C9-C7-O3-C8
5	A	607	MYX	C6-C5-C7-O3
2	B	601	FAD	PA-O3P-P-O5'
5	B	607	MYX	C18-C17-C19-C20
5	A	607	MYX	C18-C17-C19-C20
5	A	607	MYX	O1-C1-C2-C3
4	A	606	MES	C7-C8-S-O2S
5	B	607	MYX	C5-C7-C9-C10
5	A	607	MYX	C21-C22-C23-C24
2	A	601	FAD	O4B-C4B-C5B-O5B

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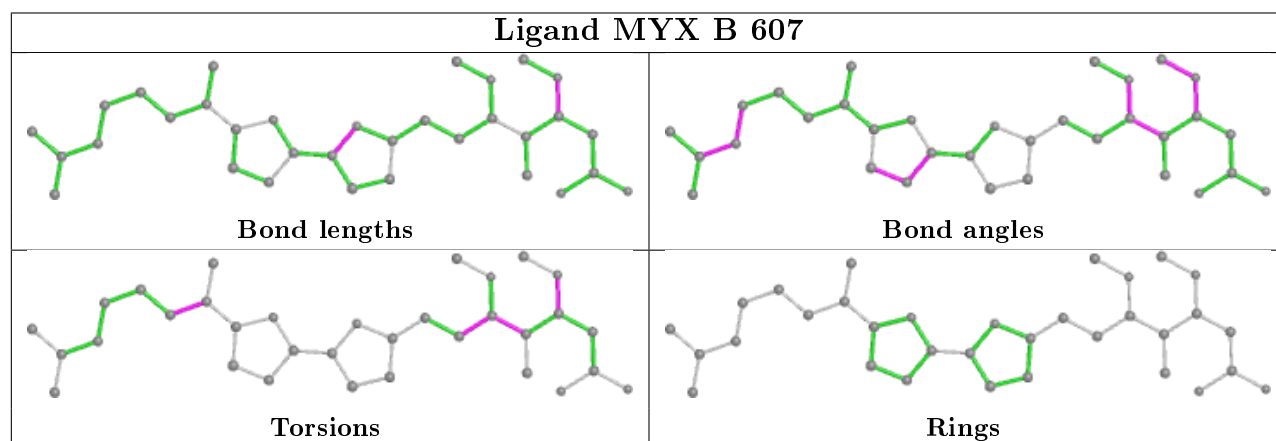
Mol	Chain	Res	Type	Atoms
5	A	607	MYX	C2-C3-C5-C6
5	A	607	MYX	C21-C22-C23-C25
5	A	607	MYX	C5-C7-O3-C8
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O3'-C3'-C4'-C5'
5	A	607	MYX	C1-C2-C3-O2

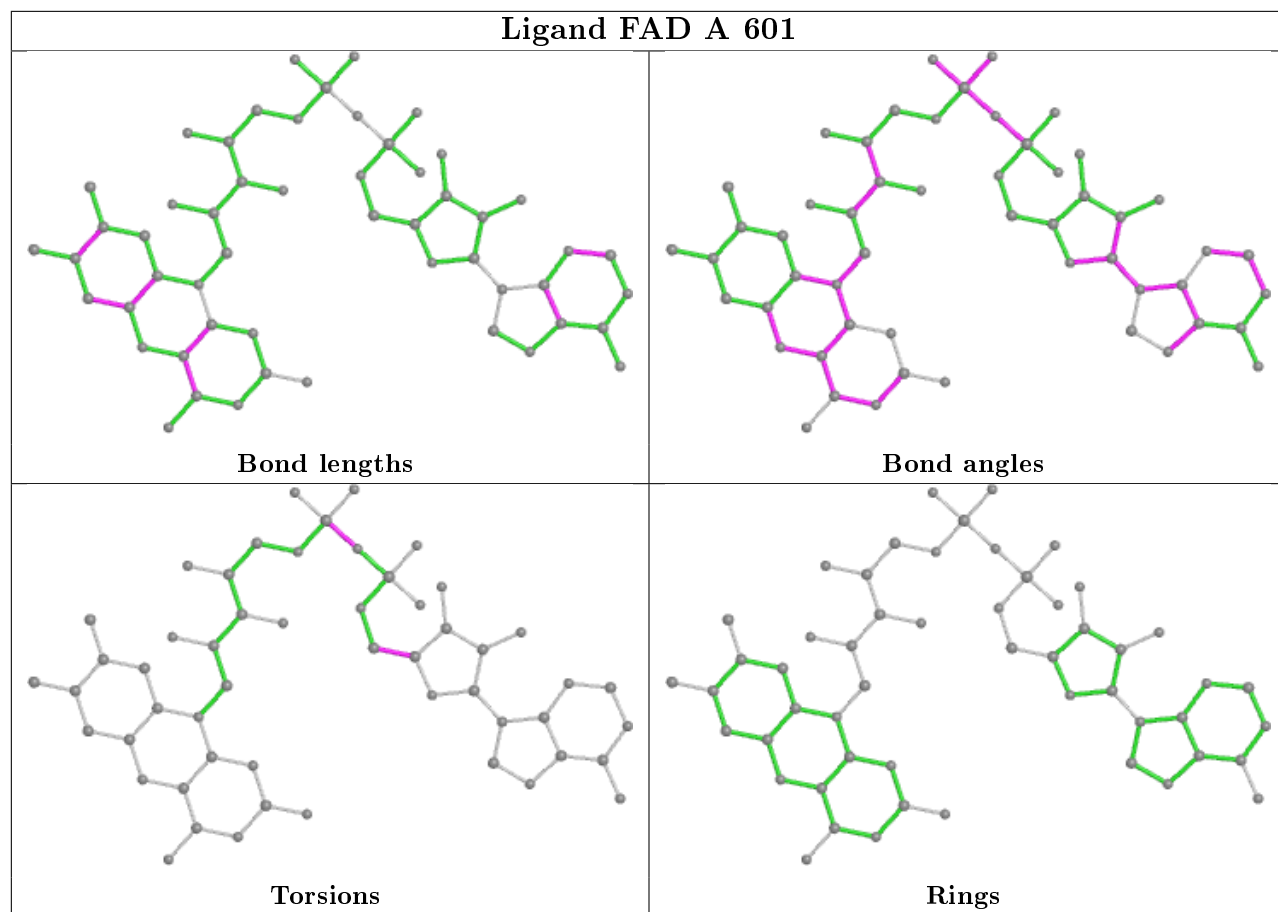
There are no ring outliers.

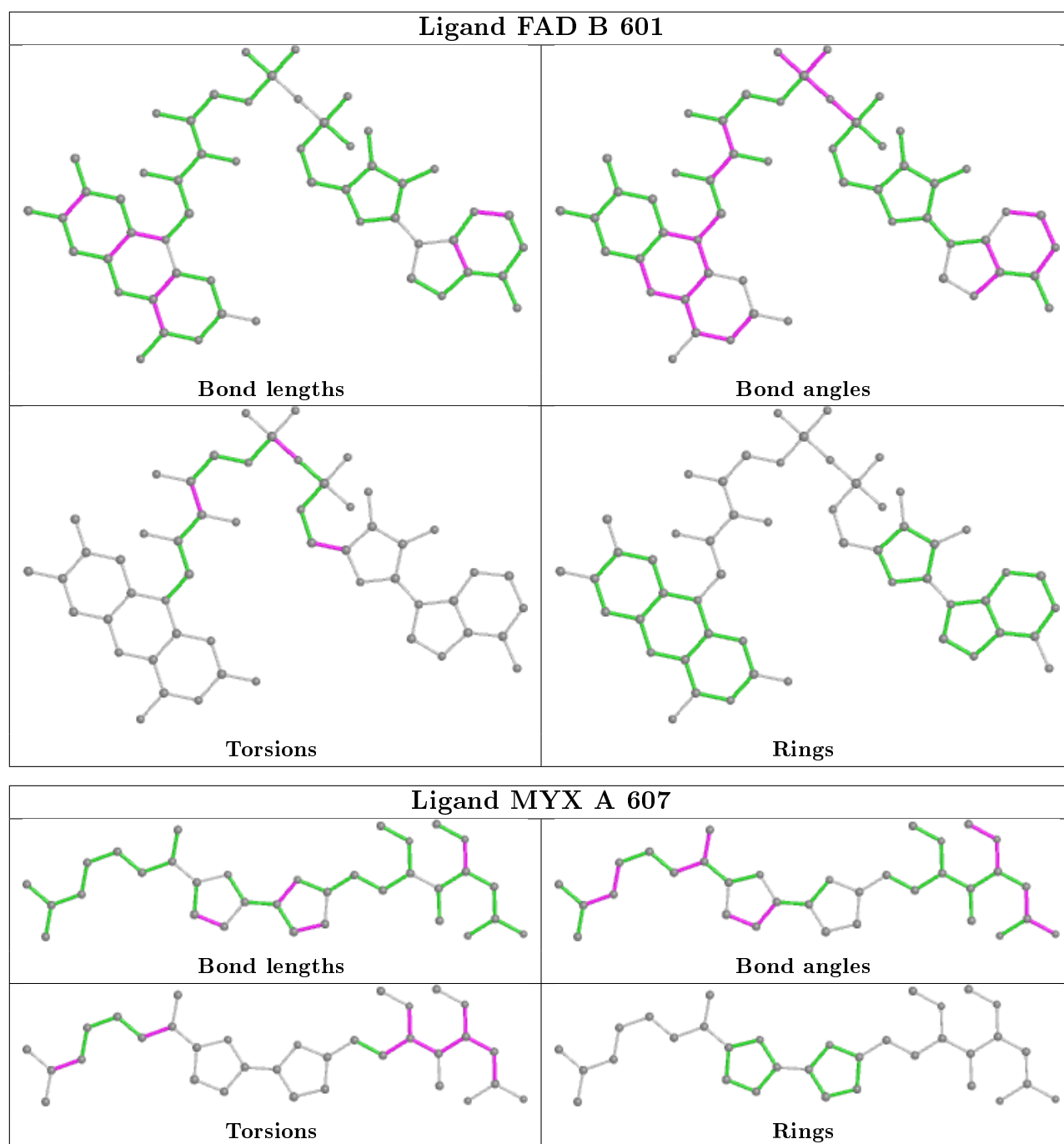
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	607	MYX	1	0
2	A	601	FAD	1	0
2	B	601	FAD	1	0
5	A	607	MYX	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	464/486 (95%)	-0.21	14 (3%)	50 36	39, 82, 138, 179	0
1	B	464/486 (95%)	-0.18	17 (3%)	41 28	41, 86, 128, 199	0
All	All	928/972 (95%)	-0.20	31 (3%)	46 32	39, 84, 134, 199	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	7.9
1	B	145	SER	6.9
1	A	33	SER	6.9
1	B	46	ILE	6.8
1	B	30	VAL	6.4
1	B	45	VAL	6.1
1	A	50	HIS	5.7
1	B	47	ASP	5.5
1	A	46	ILE	5.0
1	B	425	ASP	4.3
1	A	51	SER	4.3
1	B	50	HIS	4.1
1	B	426	LYS	4.0
1	B	51	SER	3.5
1	B	427	ILE	3.5
1	A	425	ASP	3.4
1	B	34	GLY	3.4
1	B	144	LEU	3.1
1	A	47	ASP	3.0
1	A	45	VAL	3.0
1	A	426	LYS	2.9
1	B	48	PRO	2.8
1	A	145	SER	2.8
1	B	49	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	464	ARG	2.7
1	B	319	LYS	2.5
1	B	419	ASN	2.5
1	A	44	LYS	2.5
1	B	135	ASP	2.3
1	A	52	ASP	2.0
1	A	144	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

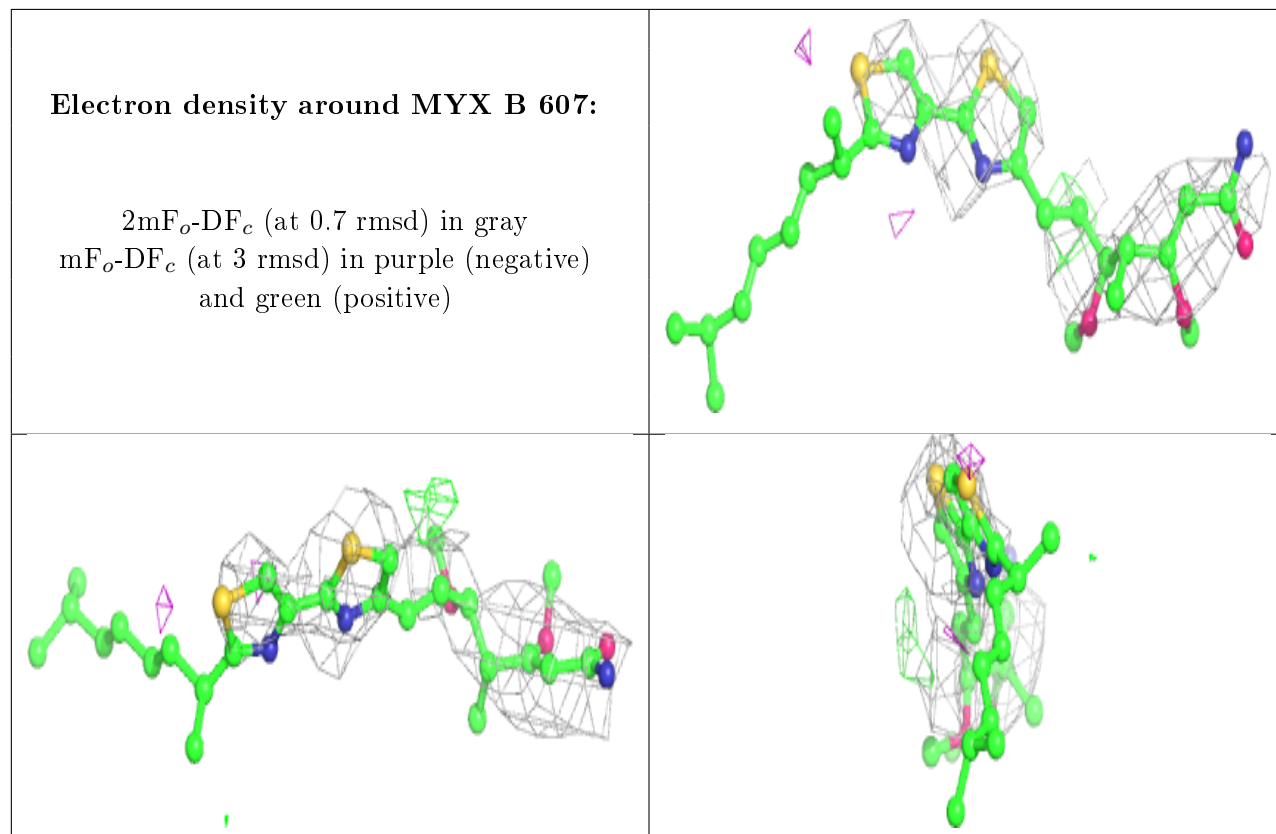
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MYX	B	607	33/33	0.74	0.44	127,164,188,190	0
5	MYX	A	607	33/33	0.77	0.37	125,140,167,168	0
3	MG	A	604	1/1	0.83	0.38	77,77,77,77	0
4	MES	A	606	12/12	0.90	0.24	125,130,141,145	0
4	MES	B	606	12/12	0.92	0.20	123,127,146,146	0
3	MG	B	605	1/1	0.94	0.33	65,65,65,65	0
3	MG	A	603	1/1	0.94	0.12	92,92,92,92	0
3	MG	B	603	1/1	0.96	0.49	72,72,72,72	0
3	MG	B	602	1/1	0.96	0.33	88,88,88,88	0
2	FAD	B	601	53/53	0.97	0.14	46,59,85,93	0
3	MG	B	604	1/1	0.98	0.25	81,81,81,81	0
2	FAD	A	601	53/53	0.98	0.14	44,55,84,91	0
3	MG	A	602	1/1	0.98	0.23	69,69,69,69	0
3	MG	A	605	1/1	0.99	0.09	57,57,57,57	0

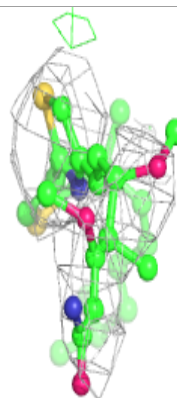
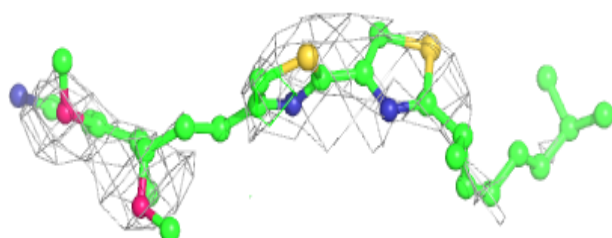
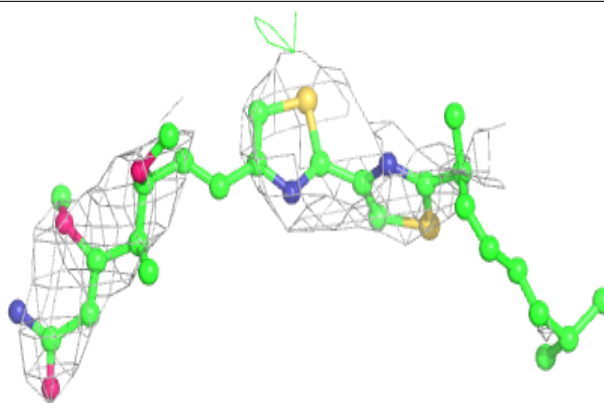
The following is a graphical depiction of the model fit to experimental electron density of all

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.

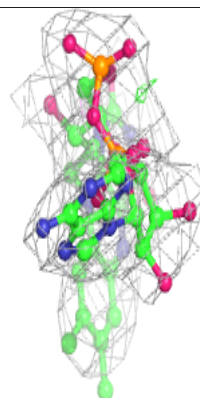
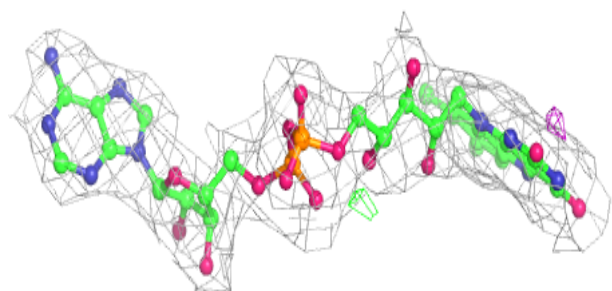
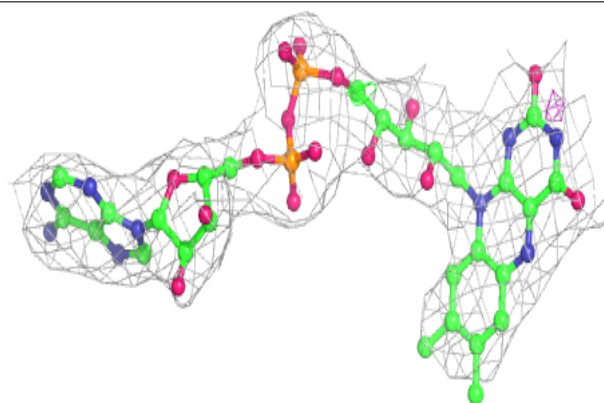


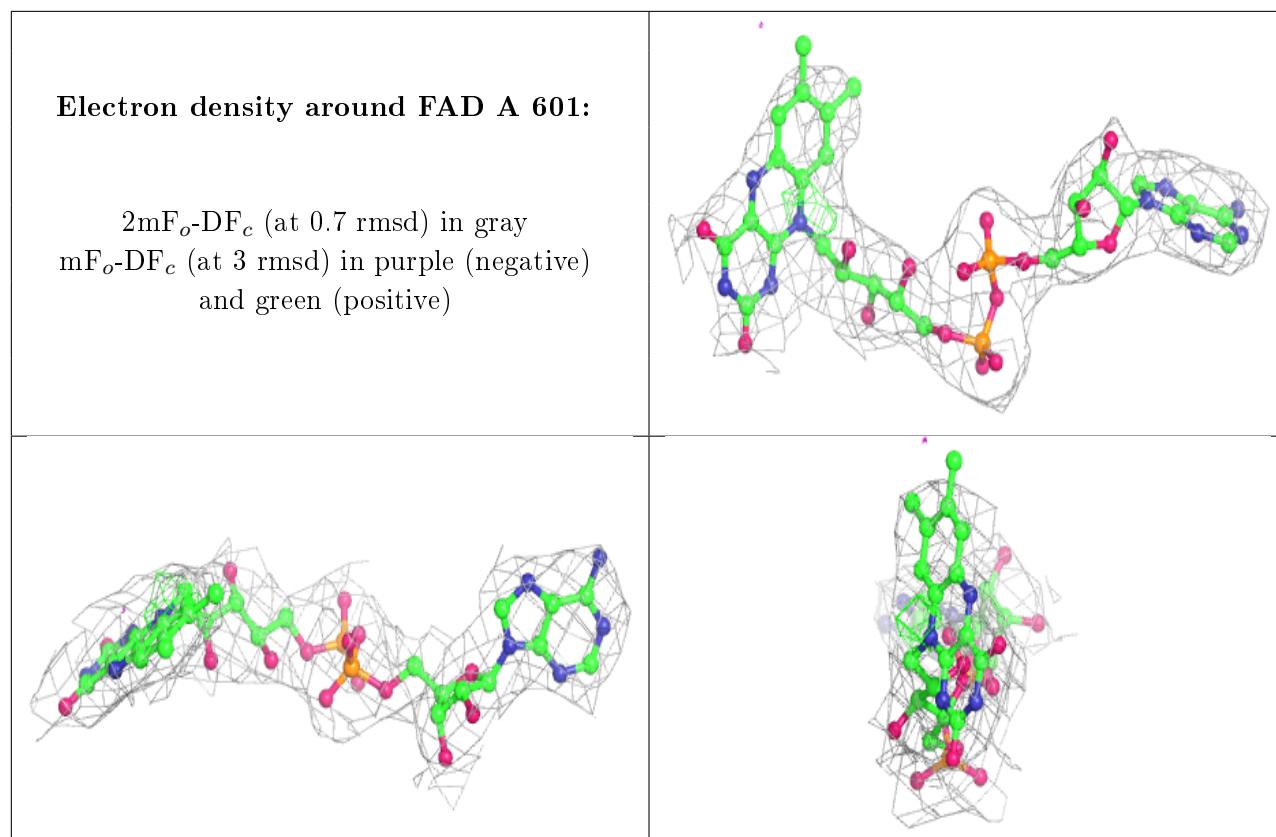
Electron density around MYX A 607:

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

**Electron density around FAD B 601:**

$2mF_o-DF_c$ (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.