



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 1, 2025 – 10:56 pm BST

PDB ID : 6FCX / pdb_00006fcx
Title : Structure of human 5,10-methylenetetrahydrofolate reductase (MTHFR)
Authors : Kopec, J.; Bezerra, G.A.; Oberholzer, A.E.; Rembeza, E.; Sorrell, F.J.; Chalk, R.; Borkowska, O.; Ellis, K.; Kupinska, K.; Krojer, T.; Burgess-Brown, N.; Von Delft, F.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Froese, D.S.; Baumgartner, M.; Yue, W.W.; Structural Genomics Consortium (SGC)
Deposited on : 2017-12-21
Resolution : 2.50 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

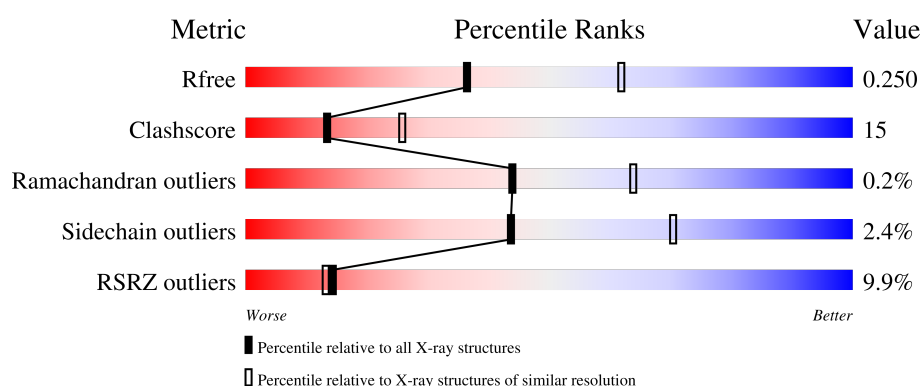
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	615	<div> <div>3%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	B	615	<div> <div>16%</div> <div>73%</div> <div>21%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9180 atoms, of which 10 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 Methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4723	3048	786	870	19			
1	B	590	Total	C	N	O	S	0	0	0
			4191	2660	727	791	13			

There are 20 discrepancies between the modelled and reference sequences:

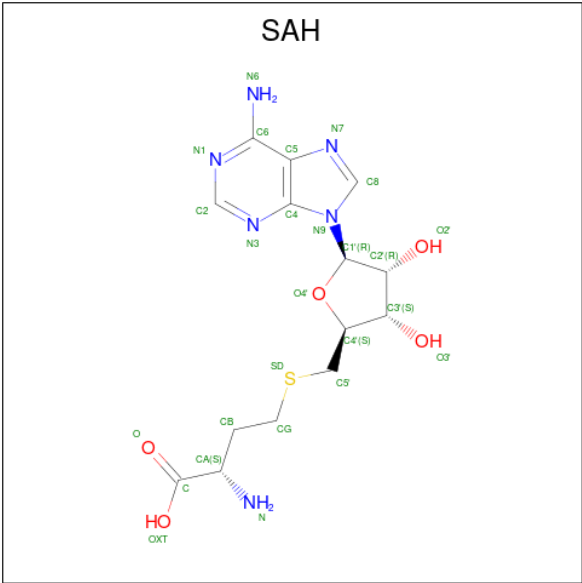
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	LEU	initiating methionine	UNP P42898
A	429	ALA	GLU	variant	UNP P42898
A	594	GLN	ARG	variant	UNP P42898
A	645	ALA	-	expression tag	UNP P42898
A	646	GLU	-	expression tag	UNP P42898
A	647	ASN	-	expression tag	UNP P42898
A	648	LEU	-	expression tag	UNP P42898
A	649	TYR	-	expression tag	UNP P42898
A	650	PHE	-	expression tag	UNP P42898
A	651	GLN	-	expression tag	UNP P42898
B	37	MET	LEU	initiating methionine	UNP P42898
B	429	ALA	GLU	variant	UNP P42898
B	594	GLN	ARG	variant	UNP P42898
B	645	ALA	-	expression tag	UNP P42898
B	646	GLU	-	expression tag	UNP P42898
B	647	ASN	-	expression tag	UNP P42898
B	648	LEU	-	expression tag	UNP P42898
B	649	TYR	-	expression tag	UNP P42898
B	650	PHE	-	expression tag	UNP P42898
B	651	GLN	-	expression tag	UNP P42898

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



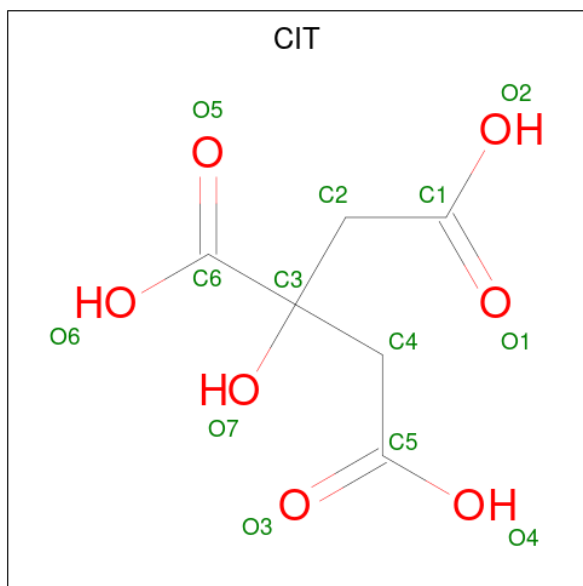
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			18	6	5	7		
4	B	1	Total	C	H	O	0	0
			18	6	5	7		

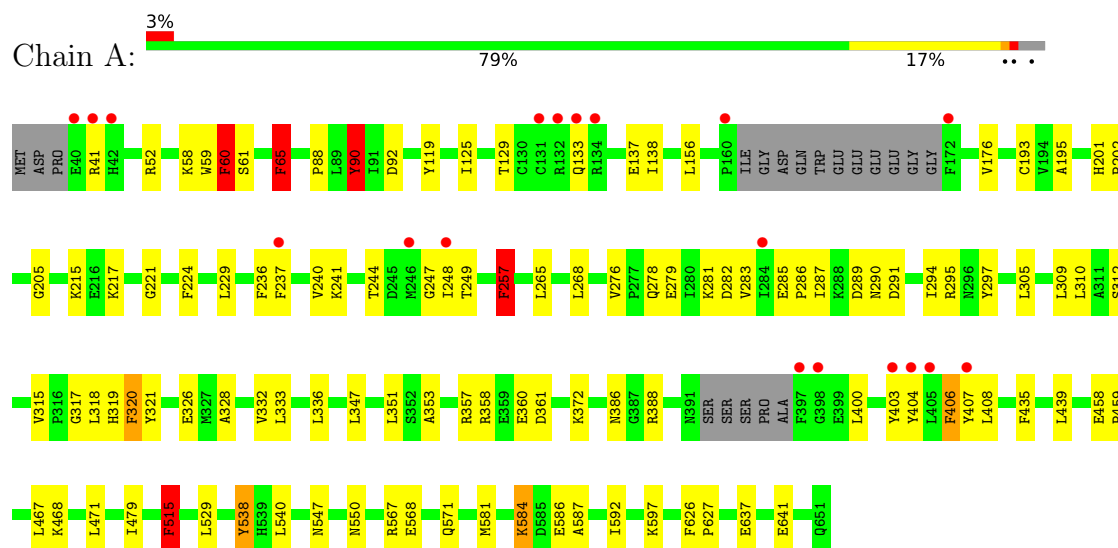
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	24	Total	O	0	0
			24	24		

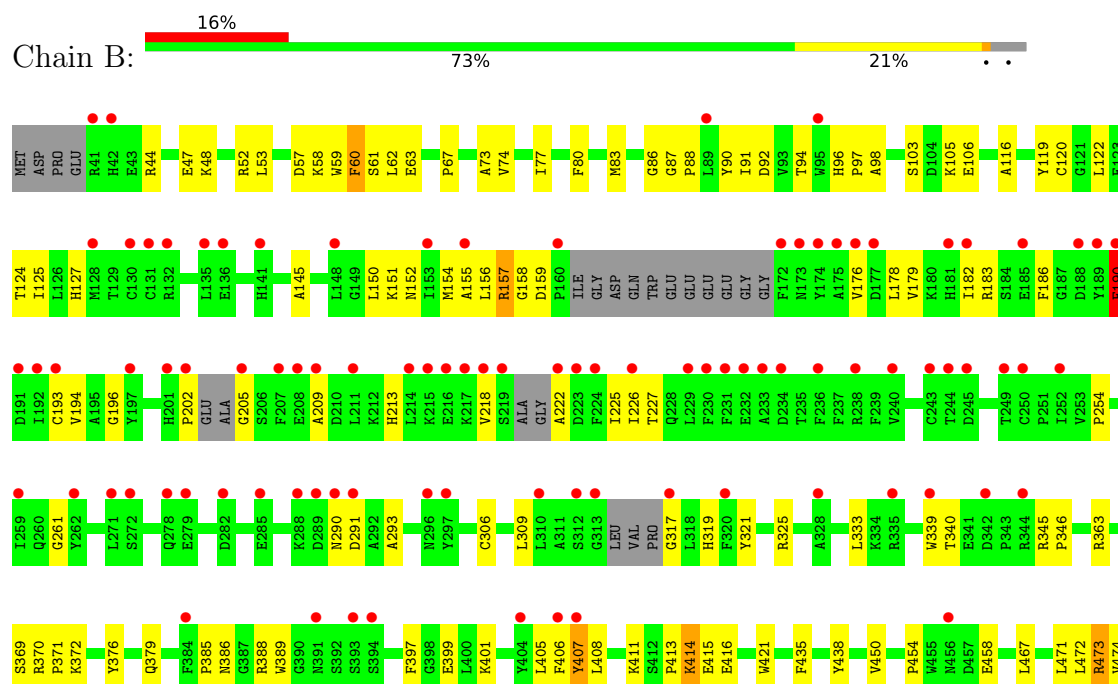
3 Residue-property plots

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: Methylenetetrahydrofolate reductase



• Molecule 1: Methylenetetrahydrofolate reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.34Å 127.94Å 147.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.97 – 2.50 63.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.97-2.50) 100.0 (63.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.210 , 0.247 0.215 , 0.250	Depositor DCC
R_{free} test set	3266 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9180	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CIT, SAH

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	0.65	0/4853	0.83	13/6606 (0.2%)
1	B	0.55	0/4295	0.70	5/5885 (0.1%)
All	All	0.61	0/9148	0.77	18/12491 (0.1%)

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	A	0	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	TYR	CB-CG-CD2	-9.15	115.51	121.00
1	B	515	PHE	CB-CG-CD2	-8.94	114.55	120.80
1	A	65	PHE	CB-CG-CD2	-8.56	114.81	120.80
1	A	60	PHE	CB-CG-CD2	-7.69	115.42	120.80
1	A	515	PHE	CB-CG-CD2	-7.60	115.48	120.80
1	A	361	ASP	CB-CG-OD1	7.41	124.97	118.30
1	B	515	PHE	CB-CG-CD1	6.62	125.43	120.80
1	A	515	PHE	CB-CG-CD1	6.52	125.36	120.80
1	A	65	PHE	CB-CG-CD1	6.36	125.25	120.80
1	A	90	TYR	CB-CG-CD1	6.33	124.80	121.00
1	A	400	LEU	CB-CG-CD2	5.64	120.60	111.00
1	B	190	PHE	CB-CG-CD1	5.57	124.70	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	PHE	CB-CG-CD1	5.50	124.65	120.80
1	B	538	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	B	363	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	257	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	A	90	TYR	CA-CB-CG	5.19	123.27	113.40
1	A	361	ASP	CB-CG-OD2	-5.05	113.75	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	TYR	Peptide
1	A	515	PHE	Sidechain
1	A	60	PHE	Sidechain
1	A	65	PHE	Sidechain
1	A	90	TYR	Sidechain
1	B	515	PHE	Sidechain
1	B	538	TYR	Sidechain

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	4723	0	4516	120	0
1	B	4191	0	3577	140	0
2	A	53	0	31	3	0
2	B	53	0	30	2	0
3	A	26	0	19	0	0
3	B	26	0	17	0	0
4	A	13	5	5	1	0
4	B	13	5	5	1	0
5	A	48	0	0	0	0
5	B	24	0	0	2	0
All	All	9170	10	8200	251	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 15.

All (251) 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:B:62:LEU:HB2	1:B:91:ILE:HD11	1.31	1.11
1:B:62:LEU:HB2	1:B:91:ILE:CD1	1.81	1.09
1:A:529:LEU:HD13	1:A:538:TYR:CD2	1.92	1.05
1:A:439:LEU:O	1:A:468:LYS:NZ	1.93	0.99
1:B:157:ARG:HB3	2:B:701:FAD:H5'1	1.44	0.99
1:B:411:LYS:NZ	1:B:458:GLU:OE2	1.95	0.98
1:B:61:SER:HB3	1:B:319:HIS:HA	1.48	0.94
1:B:529:LEU:HD13	1:B:538:TYR:CD2	2.03	0.93
1:A:571:GLN:O	1:A:571:GLN:HG3	1.67	0.92
1:A:529:LEU:HD13	1:A:538:TYR:HD2	1.29	0.92
1:A:276:VAL:HG13	1:A:281:LYS:HD2	1.53	0.91
1:A:567:ARG:HG2	1:B:555:GLN:HE21	1.35	0.90
1:A:92:ASP:OD1	1:A:125:ILE:HB	1.72	0.87
1:A:357:ARG:HD3	1:A:360:GLU:OE2	1.75	0.86
1:A:215:LYS:HA	1:A:248:ILE:HD11	1.58	0.84
1:A:567:ARG:HG2	1:B:555:GLN:NE2	1.93	0.82
1:A:129:THR:HG22	1:A:156:LEU:HB2	1.61	0.82
1:B:159:ASP:OD1	2:B:701:FAD:O4'	2.00	0.79
1:B:405:LEU:HD13	1:B:407:TYR:HE1	1.48	0.79
1:B:190:PHE:HD1	1:B:190:PHE:O	1.65	0.78
1:B:154:MET:HG2	1:B:156:LEU:CD1	2.14	0.77
1:B:571:GLN:O	1:B:571:GLN:HG3	1.83	0.77
1:A:332:VAL:O	1:A:336:LEU:HD13	1.84	0.77
1:A:318:LEU:HB3	1:A:320:PHE:HE1	1.50	0.76
1:A:201:HIS:CD2	1:A:202:PRO:HD2	2.22	0.75
1:B:529:LEU:HD13	1:B:538:TYR:HD2	1.52	0.74
1:B:53:LEU:HG	1:B:59:TRP:CZ3	2.24	0.72
1:A:283:VAL:HG21	1:A:297:TYR:CZ	2.25	0.71
1:A:215:LYS:HA	1:A:248:ILE:CD1	2.20	0.71
1:B:62:LEU:CB	1:B:91:ILE:HD11	2.15	0.71
1:B:538:TYR:O	1:B:538:TYR:HD1	1.74	0.71
1:B:218:VAL:O	1:B:222:ALA:HB3	1.91	0.70
1:A:129:THR:HG22	1:A:156:LEU:CB	2.22	0.70
1:A:626:PHE:CG	1:A:627:PRO:HD3	2.27	0.69
1:A:290:ASN:O	1:A:294:ILE:HD12	1.91	0.69
1:B:515:PHE:CZ	1:B:619:VAL:HG21	2.28	0.69
1:B:476:ARG:NH1	5:B:801:HOH:O	2.25	0.68
1:B:435:PHE:CE2	1:B:480:LEU:HB3	2.27	0.68
1:A:156:LEU:HD13	2:A:701:FAD:C4X	2.24	0.67
1:B:438:TYR:HA	1:B:450:VAL:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HB3	1:A:320:PHE:CE1	2.29	0.67
1:B:154:MET:CE	1:B:156:LEU:HD11	2.26	0.66
1:A:406:PHE:HE1	1:A:407:TYR:CE2	2.15	0.65
1:B:346:PRO:HD2	5:B:806:HOH:O	1.97	0.64
1:B:405:LEU:HD13	1:B:407:TYR:CE1	2.31	0.64
1:A:58:LYS:HG3	1:A:310:LEU:HD12	1.79	0.64
1:A:568:GLU:OE2	1:B:556:PRO:HG2	1.98	0.64
1:B:145:ALA:O	1:B:150:LEU:HB2	1.99	0.63
1:B:125:ILE:HA	1:B:152:ASN:O	1.98	0.63
1:B:60:PHE:HZ	1:B:333:LEU:CB	2.12	0.63
1:A:41:ARG:O	1:A:41:ARG:HG3	1.99	0.62
1:A:58:LYS:HE3	1:A:315:VAL:O	2.00	0.62
1:B:413:PRO:HG2	1:B:416:GLU:HG2	1.80	0.62
1:B:90:TYR:HD2	1:B:125:ILE:CD1	2.12	0.62
1:B:472:LEU:O	1:B:476:ARG:HG3	2.00	0.62
1:B:155:ALA:O	1:B:156:LEU:HD12	2.00	0.62
1:A:41:ARG:NH1	1:A:52:ARG:HH21	1.97	0.61
1:A:236:PHE:O	1:A:240:VAL:HG23	1.99	0.61
1:B:92:ASP:OD2	1:B:127:HIS:NE2	2.33	0.61
1:A:283:VAL:HG21	1:A:297:TYR:CE2	2.35	0.61
1:B:626:PHE:CG	1:B:627:PRO:HD3	2.35	0.61
1:B:154:MET:HG2	1:B:156:LEU:HD11	1.83	0.61
1:B:155:ALA:C	1:B:156:LEU:HD12	2.22	0.60
1:B:438:TYR:N	1:B:450:VAL:HG21	2.16	0.60
1:B:209:ALA:O	1:B:213:HIS:N	2.32	0.60
1:B:190:PHE:O	1:B:190:PHE:CD1	2.52	0.60
1:A:279:GLU:OE1	1:A:279:GLU:N	2.26	0.60
1:B:87:GLY:N	1:B:88:PRO:HD3	2.17	0.60
1:A:41:ARG:HH12	1:A:52:ARG:NE	1.99	0.60
1:A:295:ARG:HD2	1:A:328:ALA:HB2	1.83	0.59
1:A:637:GLU:O	1:A:641:GLU:HG3	2.02	0.59
1:B:196:GLY:O	1:B:227:THR:HA	2.02	0.59
1:B:62:LEU:HD13	1:B:83:MET:HE1	1.85	0.59
1:A:119:TYR:CE2	1:A:372:LYS:HE3	2.38	0.59
1:A:241:LYS:HA	1:A:244:THR:OG1	2.03	0.59
1:A:317:GLY:O	1:A:318:LEU:HD12	2.03	0.59
1:B:397:PHE:HB2	1:B:582:PHE:CD2	2.38	0.58
1:B:405:LEU:HD12	1:B:408:LEU:HD12	1.85	0.58
1:A:41:ARG:HH12	1:A:52:ARG:CZ	2.16	0.58
1:A:215:LYS:CA	1:A:248:ILE:HD11	2.30	0.58
1:A:388:ARG:NH2	1:B:386:ASN:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HA	1:B:57:ASP:O	2.04	0.58
1:B:151:LYS:O	1:B:190:PHE:CD1	2.57	0.58
1:B:157:ARG:HD3	1:B:158:GLY:N	2.19	0.58
1:A:406:PHE:CE1	1:A:407:TYR:CE2	2.92	0.57
1:B:376:TYR:O	1:B:379:GLN:HG2	2.05	0.56
1:B:154:MET:HG3	1:B:193:CYS:O	2.05	0.56
1:B:119:TYR:CE2	1:B:407:TYR:HE2	2.24	0.56
1:A:60:PHE:CD1	1:A:60:PHE:C	2.78	0.56
1:A:247:GLY:O	1:A:249:THR:HG23	2.06	0.56
1:B:48:LYS:O	1:B:52:ARG:NE	2.39	0.56
1:A:41:ARG:NH1	1:A:52:ARG:NH2	2.54	0.56
1:B:60:PHE:CZ	1:B:333:LEU:CB	2.88	0.55
1:B:119:TYR:CE2	1:B:407:TYR:CE2	2.94	0.55
1:B:106:GLU:OE1	1:B:406:PHE:HB3	2.07	0.55
1:A:52:ARG:HH11	1:A:59:TRP:HB3	1.71	0.54
1:B:182:ILE:O	1:B:186:PHE:N	2.40	0.54
1:B:155:ALA:HB1	1:B:178:LEU:CB	2.37	0.54
1:B:399:GLU:OE1	1:B:401:LYS:HE3	2.08	0.54
1:B:48:LYS:O	1:B:52:ARG:CD	2.56	0.54
1:B:405:LEU:HB3	1:B:407:TYR:CE1	2.42	0.54
1:A:276:VAL:O	1:A:281:LYS:HD2	2.08	0.53
1:B:90:TYR:CD2	1:B:125:ILE:CD1	2.92	0.53
1:B:306:CYS:HA	1:B:309:LEU:CB	2.38	0.53
1:A:281:LYS:O	1:A:285:GLU:HG2	2.08	0.53
1:A:309:LEU:O	1:A:312:SER:HB3	2.08	0.53
1:B:190:PHE:CD1	1:B:190:PHE:C	2.82	0.53
1:A:279:GLU:H	1:A:279:GLU:CD	2.12	0.53
1:A:41:ARG:HH12	1:A:52:ARG:NH2	2.05	0.53
1:A:65:PHE:CD1	1:A:65:PHE:C	2.83	0.53
1:B:450:VAL:HG23	1:B:450:VAL:O	2.09	0.53
1:A:265:LEU:HA	1:A:268:LEU:CD2	2.39	0.52
1:A:439:LEU:O	1:A:468:LYS:CE	2.58	0.52
1:B:515:PHE:CZ	1:B:619:VAL:CG2	2.93	0.52
1:B:59:TRP:CD1	1:B:317:GLY:HA3	2.44	0.52
1:B:62:LEU:HD13	1:B:83:MET:CE	2.39	0.52
1:B:96:HIS:CD2	1:B:98:ALA:HB3	2.45	0.51
1:B:438:TYR:HA	1:B:450:VAL:CG2	2.40	0.51
1:A:581:MET:O	1:A:584:LYS:HE3	2.09	0.51
1:A:133:GLN:HB3	1:A:138:ILE:HD11	1.93	0.51
1:B:62:LEU:HB2	1:B:91:ILE:HD12	1.82	0.51
1:A:133:GLN:HA	1:A:137:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLY:N	1:B:226:ILE:O	2.39	0.50
1:A:92:ASP:OD2	1:A:319:HIS:HE1	1.93	0.50
1:B:91:ILE:HG13	1:B:92:ASP:H	1.77	0.50
1:B:67:PRO:HG3	1:B:73:ALA:HA	1.93	0.49
1:A:265:LEU:O	1:A:268:LEU:HD23	2.12	0.49
1:B:421:TRP:CZ2	1:B:454:PRO:HD3	2.48	0.49
1:A:278:GLN:O	1:A:282:ASP:N	2.36	0.49
1:A:567:ARG:NH1	1:B:555:GLN:HE22	2.11	0.48
1:A:626:PHE:CD2	1:A:627:PRO:HD3	2.47	0.48
1:B:86:GLY:HA3	1:B:339:TRP:NE1	2.28	0.48
1:A:236:PHE:CE2	1:A:315:VAL:HG12	2.48	0.48
1:A:279:GLU:O	1:A:283:VAL:HG13	2.12	0.48
1:A:538:TYR:HD1	1:A:538:TYR:O	1.97	0.48
1:A:538:TYR:HE1	1:A:550:ASN:N	2.11	0.48
1:A:133:GLN:CB	1:A:138:ILE:HD11	2.44	0.48
1:A:479:ILE:HG23	1:A:515:PHE:CG	2.49	0.48
1:A:61:SER:HB2	1:A:90:TYR:CD1	2.49	0.48
1:A:567:ARG:HH11	1:B:555:GLN:HE22	1.61	0.48
1:B:96:HIS:HD2	1:B:98:ALA:HB3	1.79	0.47
1:B:515:PHE:CD1	1:B:515:PHE:C	2.87	0.47
1:B:407:TYR:HD1	1:B:407:TYR:H	1.62	0.47
1:A:119:TYR:CD2	1:A:372:LYS:HE3	2.49	0.47
1:B:176:VAL:O	1:B:178:LEU:N	2.39	0.47
1:A:467:LEU:CD1	1:A:471:LEU:CD1	2.92	0.47
1:A:229:LEU:C	1:A:229:LEU:HD12	2.35	0.47
1:A:406:PHE:CE1	1:A:407:TYR:CD2	3.02	0.47
1:B:369:SER:C	1:B:371:PRO:HD3	2.34	0.47
1:A:60:PHE:C	1:A:60:PHE:HD1	2.17	0.46
1:B:370:ARG:N	1:B:371:PRO:HD3	2.30	0.46
1:A:276:VAL:HG22	1:A:281:LYS:HG3	1.96	0.46
1:B:74:VAL:HG12	1:B:406:PHE:O	2.15	0.46
1:B:435:PHE:CD2	1:B:480:LEU:HB3	2.50	0.46
1:B:90:TYR:HD2	1:B:125:ILE:HD13	1.78	0.46
1:A:41:ARG:HH12	1:A:52:ARG:HE	1.63	0.46
1:B:94:THR:HA	1:B:127:HIS:ND1	2.31	0.46
1:A:257:PHE:HB2	1:A:321:TYR:HD2	1.80	0.46
1:A:467:LEU:HD13	1:A:471:LEU:HG	1.97	0.46
1:B:584:LYS:HG3	1:B:585:ASP:N	2.31	0.46
1:A:283:VAL:CG2	1:A:297:TYR:CE2	3.00	0.45
1:B:202:PRO:HA	1:B:205:GLY:N	2.32	0.45
1:A:353:ALA:HA	1:A:358:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:TYR:CD1	1:B:538:TYR:C	2.90	0.45
1:A:60:PHE:CE1	1:A:88:PRO:HB3	2.52	0.45
1:A:201:HIS:CG	1:A:202:PRO:HD2	2.49	0.45
1:A:347:LEU:HD12	1:A:351:LEU:HD21	1.98	0.45
1:A:406:PHE:HE1	1:A:407:TYR:CZ	2.35	0.45
1:B:421:TRP:CH2	1:B:454:PRO:HD3	2.52	0.45
1:A:406:PHE:HE1	1:A:407:TYR:CD2	2.34	0.45
1:B:59:TRP:O	1:B:317:GLY:HA2	2.17	0.45
1:B:405:LEU:CD1	1:B:407:TYR:HE1	2.24	0.45
1:B:405:LEU:HB3	1:B:407:TYR:CD1	2.52	0.44
1:B:467:LEU:HD12	1:B:471:LEU:CD1	2.46	0.44
1:B:473:ARG:NE	1:B:637:GLU:OE2	2.48	0.44
1:B:538:TYR:HD1	1:B:538:TYR:C	2.20	0.44
1:A:538:TYR:CE1	1:A:550:ASN:N	2.85	0.44
1:B:73:ALA:O	1:B:77:ILE:HG12	2.16	0.44
1:A:156:LEU:HD13	2:A:701:FAD:C4	2.47	0.44
1:A:592:ILE:O	1:A:597:LYS:HG2	2.18	0.44
1:B:145:ALA:C	1:B:150:LEU:HB2	2.38	0.44
1:B:53:LEU:HD23	1:B:57:ASP:O	2.17	0.44
1:B:59:TRP:NE1	1:B:317:GLY:HA3	2.33	0.44
1:A:65:PHE:C	1:A:65:PHE:HD1	2.20	0.44
1:A:406:PHE:CD1	1:A:406:PHE:C	2.90	0.44
1:B:120:CYS:HB3	1:B:122:LEU:HD23	2.00	0.44
1:B:254:PRO:HD2	1:B:317:GLY:O	2.18	0.44
1:B:509:GLN:HG2	1:B:560:THR:HG23	2.00	0.44
1:B:519:ARG:HG3	1:B:617:PHE:HE1	1.83	0.44
1:A:195:ALA:HB1	2:A:701:FAD:HM83	2.00	0.43
1:A:305:LEU:HD23	1:A:309:LEU:HG	2.00	0.43
1:A:626:PHE:CD1	1:A:627:PRO:HD3	2.53	0.43
1:B:155:ALA:CB	1:B:178:LEU:CB	2.96	0.43
1:B:340:THR:HG23	1:B:340:THR:O	2.18	0.43
1:A:236:PHE:HE2	1:A:315:VAL:HG12	1.83	0.43
1:A:278:GLN:HA	1:A:281:LYS:HB2	1.99	0.43
1:A:538:TYR:CE1	1:A:550:ASN:HB3	2.52	0.43
1:B:119:TYR:O	1:B:372:LYS:HE3	2.18	0.43
1:B:183:ARG:HA	1:B:186:PHE:CB	2.48	0.43
1:A:467:LEU:CD1	1:A:471:LEU:HD11	2.49	0.43
1:A:291:ASP:HA	1:A:294:ILE:HD13	2.01	0.43
1:B:261:GLY:HA2	1:B:291:ASP:CB	2.49	0.43
1:B:154:MET:HE2	1:B:156:LEU:HD11	1.99	0.43
1:B:194:VAL:O	1:B:225:ILE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:CB	1:B:47:GLU:OE1	2.66	0.43
1:B:91:ILE:HG22	1:B:124:THR:HG22	2.01	0.43
1:B:345:ARG:HA	1:B:346:PRO:HD3	1.92	0.42
1:A:257:PHE:CD1	1:A:257:PHE:C	2.92	0.42
1:B:106:GLU:HB2	1:B:406:PHE:CD1	2.54	0.42
1:A:458:GLU:HB3	1:A:459:PRO:CD	2.50	0.42
1:B:96:HIS:ND1	1:B:97:PRO:HD2	2.34	0.42
1:A:276:VAL:HG13	1:A:281:LYS:CD	2.36	0.42
1:A:403:TYR:HE2	1:A:408:LEU:HD11	1.84	0.42
1:A:571:GLN:NE2	1:B:568:GLU:OE1	2.48	0.42
1:B:399:GLU:OE1	1:B:401:LYS:CE	2.66	0.42
1:A:568:GLU:OE1	1:B:571:GLN:NE2	2.51	0.42
1:B:474:VAL:HG12	1:B:636:VAL:HG11	2.02	0.42
1:B:179:VAL:O	1:B:183:ARG:CB	2.68	0.42
1:A:257:PHE:C	1:A:257:PHE:HD1	2.23	0.42
1:B:90:TYR:CD2	1:B:125:ILE:HD13	2.54	0.42
1:B:290:ASN:O	1:B:293:ALA:N	2.53	0.42
1:B:63:GLU:OE1	1:B:321:TYR:CE1	2.73	0.41
1:B:77:ILE:O	1:B:80:PHE:HB2	2.20	0.41
1:B:386:ASN:OD1	1:B:386:ASN:C	2.58	0.41
1:A:467:LEU:HD11	1:A:471:LEU:HD11	2.01	0.41
1:A:540:LEU:O	1:A:547:ASN:HA	2.20	0.41
1:A:529:LEU:CD1	1:A:538:TYR:HD2	2.16	0.41
1:B:103:SER:OG	1:B:105:LYS:CG	2.69	0.41
1:A:265:LEU:HA	1:A:265:LEU:HD23	1.71	0.41
1:B:91:ILE:HD12	1:B:91:ILE:HA	1.77	0.41
1:B:414:LYS:HE3	1:B:415:GLU:OE2	2.21	0.41
1:A:237:PHE:CZ	1:A:312:SER:HB2	2.56	0.41
1:A:65:PHE:CD1	1:A:65:PHE:O	2.74	0.41
1:A:317:GLY:C	1:A:318:LEU:HD12	2.41	0.41
1:B:60:PHE:HD1	1:B:60:PHE:HA	1.61	0.41
1:B:385:PRO:HG2	1:B:389:TRP:CZ3	2.56	0.41
1:A:282:ASP:O	1:A:286:PRO:CD	2.69	0.41
1:A:287:ILE:O	1:A:289:ASP:N	2.54	0.41
1:A:386:ASN:OD1	1:B:388:ARG:NH2	2.48	0.41
1:B:116:ALA:HB3	1:B:124:THR:HG21	2.02	0.41
1:A:176:VAL:HG23	1:A:217:LYS:HA	2.03	0.41
1:A:326:GLU:N	4:A:703:CIT:O3	2.45	0.41
1:B:120:CYS:O	1:B:122:LEU:HD22	2.21	0.41
1:B:154:MET:CG	1:B:156:LEU:HD11	2.50	0.41
1:A:193:CYS:HB3	1:A:224:PHE:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:O	1:A:41:ARG:CG	2.69	0.40
1:B:53:LEU:CD2	1:B:58:LYS:HA	2.51	0.40
1:B:325:ARG:HB3	4:B:703:CIT:O6	2.21	0.40
1:A:60:PHE:CE2	1:A:333:LEU:HD13	2.56	0.40
1:B:526:LEU:HD23	1:B:526:LEU:HA	1.87	0.40
1:A:586:GLU:O	1:A:587:ALA:C	2.60	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	590/615 (96%)	570 (97%)	18 (3%)	2 (0%)	37	56
1	B	580/615 (94%)	548 (94%)	32 (6%)	0	100	100
All	All	1170/1230 (95%)	1118 (96%)	50 (4%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLY
1	A	221	GLY

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	491/537 (91%)	481 (98%)	10 (2%)	50	75
1	B	358/537 (67%)	348 (97%)	10 (3%)	38	65
All	All	849/1074 (79%)	829 (98%)	20 (2%)	44	70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	PHE
1	A	65	PHE
1	A	90	TYR
1	A	257	PHE
1	A	320	PHE
1	A	406	PHE
1	A	435	PHE
1	A	515	PHE
1	A	538	TYR
1	A	584	LYS
1	B	60	PHE
1	B	157	ARG
1	B	190	PHE
1	B	407	TYR
1	B	414	LYS
1	B	473	ARG
1	B	515	PHE
1	B	538	TYR
1	B	619	VAL
1	B	620	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	HIS
1	B	477	GLN
1	B	555	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	FAD	B	701	1	53,58,58	0.46	0	68,89,89	0.58	1 (1%)
4	CIT	B	703	-	12,12,12	0.99	0	17,17,17	1.47	2 (11%)
3	SAH	A	702	-	24,28,28	1.38	4 (16%)	25,40,40	1.89	7 (28%)
4	CIT	A	703	-	12,12,12	1.04	0	17,17,17	1.72	4 (23%)
2	FAD	A	701	-	53,58,58	0.51	0	68,89,89	0.67	1 (1%)
3	SAH	B	702	1	24,28,28	1.29	2 (8%)	25,40,40	1.77	6 (24%)

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	FAD	B	701	1	-	16/30/50/50	0/6/6/6
4	CIT	B	703	-	-	7/16/16/16	-
3	SAH	A	702	-	-	0/11/31/31	0/3/3/3
4	CIT	A	703	-	-	8/16/16/16	-
2	FAD	A	701	-	-	4/30/50/50	0/6/6/6
3	SAH	B	702	1	-	3/11/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	SAH	C2-N3	4.08	1.38	1.32
3	B	702	SAH	C2-N3	3.93	1.38	1.32
3	B	702	SAH	C2-N1	3.00	1.39	1.33
3	A	702	SAH	C2-N1	2.61	1.38	1.33
3	A	702	SAH	OXT-C	-2.43	1.22	1.30
3	A	702	SAH	O4'-C1'	2.26	1.44	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	SAH	N3-C2-N1	-6.21	118.97	128.68
3	B	702	SAH	N3-C2-N1	-4.74	121.26	128.68
4	A	703	CIT	O6-C6-C3	4.01	120.01	113.05
4	B	703	CIT	O6-C6-C3	3.68	119.44	113.05
3	A	702	SAH	C5'-SD-CG	-3.00	93.27	102.27
3	B	702	SAH	O4'-C1'-C2'	-2.96	102.60	106.93
3	A	702	SAH	OXT-C-O	-2.70	117.97	124.09
4	A	703	CIT	O4-C5-C4	2.48	122.32	114.35
3	B	702	SAH	O4'-C4'-C5'	2.41	115.05	108.83
3	A	702	SAH	N6-C6-N1	2.37	123.49	118.57
3	B	702	SAH	C4'-C5'-SD	-2.33	105.43	113.78
3	A	702	SAH	O3'-C3'-C4'	-2.32	104.33	111.05
2	A	701	FAD	C5A-C6A-N6A	2.31	123.86	120.35
3	A	702	SAH	O4'-C1'-C2'	-2.25	103.64	106.93
2	B	701	FAD	C5A-C6A-N6A	2.24	123.75	120.35
3	B	702	SAH	C5'-SD-CG	-2.23	95.57	102.27
4	A	703	CIT	O7-C3-C2	-2.15	104.36	109.40
3	A	702	SAH	C5-C6-N6	-2.13	117.11	120.35
3	B	702	SAH	OXT-C-O	-2.08	119.36	124.09
4	B	703	CIT	O4-C5-O3	-2.05	118.19	123.30
4	A	703	CIT	O4-C5-O3	-2.02	118.28	123.30

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C1'-C2'-C3'-O3'
2	A	701	FAD	C1'-C2'-C3'-C4'
2	B	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C1'-C2'-C3'-C4'
2	B	701	FAD	C3'-C4'-C5'-O5'

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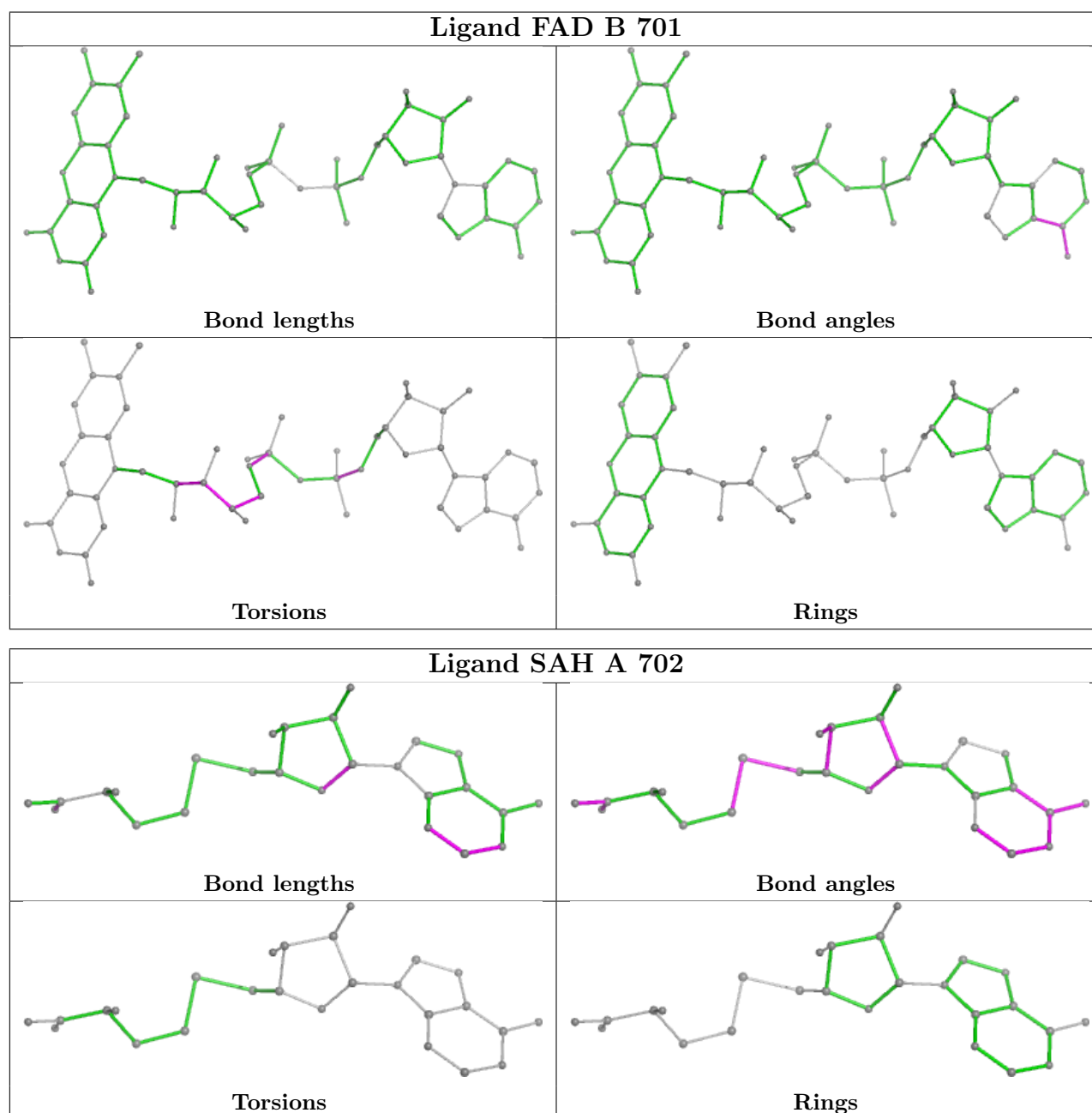
Mol	Chain	Res	Type	Atoms
2	B	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	C5'-O5'-P-O2P
2	B	701	FAD	C5'-O5'-P-O3P
3	B	702	SAH	CA-CB-CG-SD
4	A	703	CIT	C1-C2-C3-O7
4	A	703	CIT	C1-C2-C3-C4
4	A	703	CIT	C1-C2-C3-C6
4	A	703	CIT	O7-C3-C6-O5
4	B	703	CIT	O7-C3-C6-O5
4	B	703	CIT	O7-C3-C6-O6
4	B	703	CIT	C4-C3-C6-O5
4	B	703	CIT	C4-C3-C6-O6
2	A	701	FAD	O2'-C2'-C3'-C4'
2	B	701	FAD	O3'-C3'-C4'-O4'
2	B	701	FAD	C2'-C3'-C4'-O4'
4	A	703	CIT	C4-C3-C6-O5
2	B	701	FAD	O2'-C2'-C3'-C4'
4	B	703	CIT	C6-C3-C4-C5
2	B	701	FAD	C2'-C3'-C4'-C5'
4	A	703	CIT	O7-C3-C6-O6
4	A	703	CIT	C4-C3-C6-O6
2	A	701	FAD	O2'-C2'-C3'-O3'
4	B	703	CIT	C1-C2-C3-O7
2	B	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C5B-O5B-PA-O2A
2	B	701	FAD	C5'-O5'-P-O1P
2	B	701	FAD	C1'-C2'-C3'-O3'
4	B	703	CIT	C2-C3-C4-C5
3	B	702	SAH	O-C-CA-CB
3	B	702	SAH	OXT-C-CA-CB
4	A	703	CIT	C2-C3-C6-O6
2	B	701	FAD	O3'-C3'-C4'-C5'
2	B	701	FAD	O2'-C2'-C3'-O3'

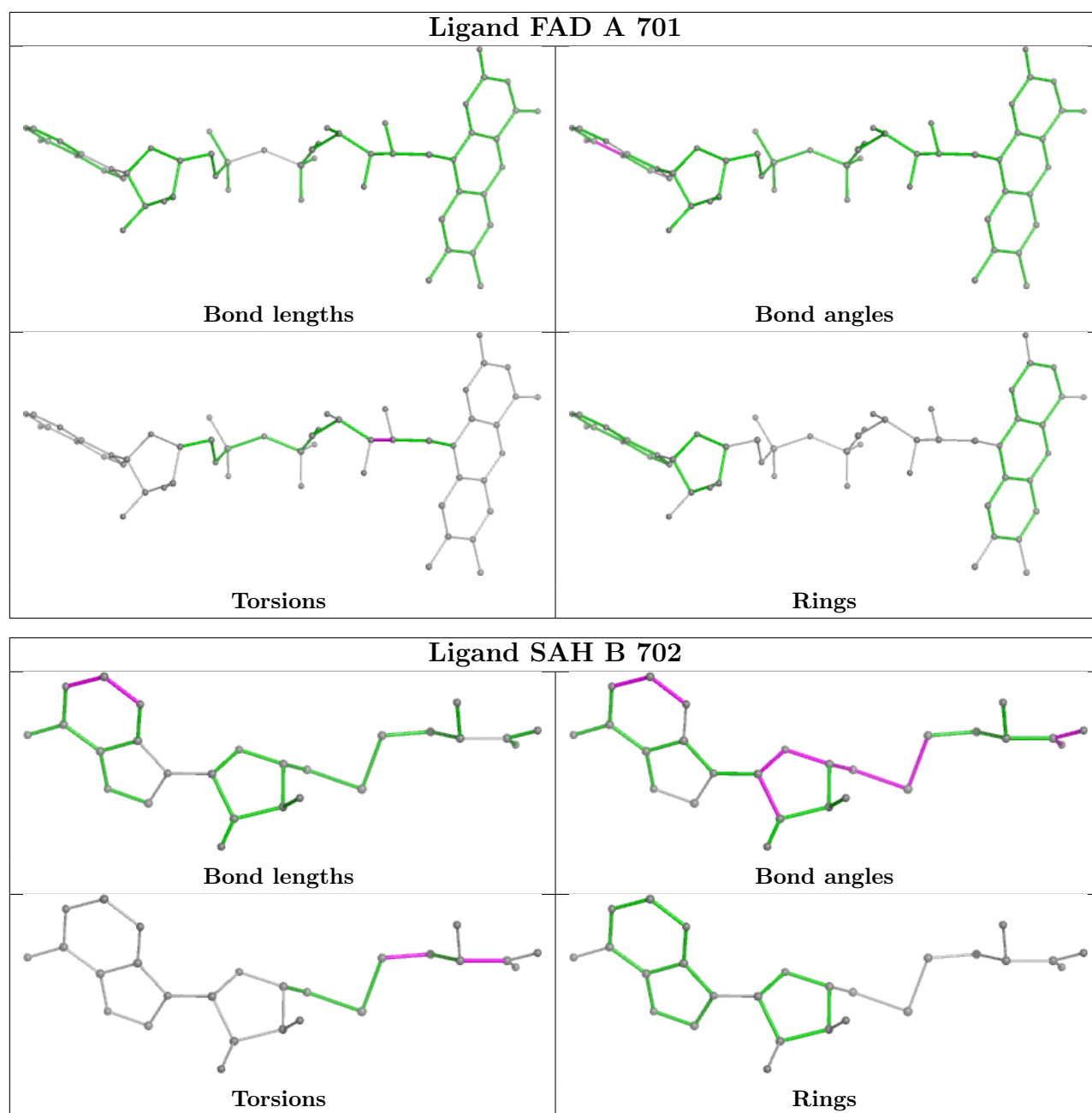
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FAD	2	0
4	B	703	CIT	1	0
4	A	703	CIT	1	0
2	A	701	FAD	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 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	596/615 (96%)	0.01	19 (3%)	50	47	48, 74, 131, 160	0
1	B	590/615 (95%)	0.77	99 (16%)	5	5	52, 97, 194, 241	0
All	All	1186/1230 (96%)	0.39	118 (9%)	14	13	48, 83, 181, 241	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	397	PHE	6.0
1	B	646	GLU	5.5
1	A	131	CYS	5.1
1	A	160	PRO	5.0
1	A	40	GLU	4.9
1	B	172	PHE	4.9
1	B	202	PRO	4.8
1	B	648	LEU	4.7
1	B	647	ASN	4.7
1	B	130	CYS	4.7
1	B	645	ALA	4.7
1	B	214	LEU	4.6
1	B	290	ASN	4.5
1	A	403	TYR	4.4
1	B	174	TYR	4.4
1	B	288	LYS	4.3
1	A	404	TYR	4.1
1	B	160	PRO	4.1
1	A	398	GLY	4.0
1	B	191	ASP	4.0
1	B	250	CYS	3.8
1	B	192	ILE	3.8
1	A	405	LEU	3.8
1	B	205	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	262	TYR	3.7
1	B	42	HIS	3.6
1	B	217	LYS	3.6
1	B	155	ALA	3.6
1	B	289	ASP	3.6
1	B	176	VAL	3.5
1	A	42	HIS	3.4
1	B	240	VAL	3.4
1	B	189	TYR	3.3
1	B	208	GLU	3.3
1	B	278	GLN	3.3
1	B	234	ASP	3.2
1	A	132	ARG	3.2
1	B	320	PHE	3.2
1	B	128	MET	3.2
1	B	197	TYR	3.2
1	B	131	CYS	3.1
1	A	246	MET	3.1
1	B	229	LEU	3.1
1	B	177	ASP	3.1
1	B	209	ALA	3.1
1	B	41	ARG	3.1
1	B	407	TYR	3.1
1	B	219	SER	3.0
1	B	89	LEU	2.9
1	B	252	ILE	2.8
1	B	233	ALA	2.8
1	B	185	GLU	2.8
1	B	224	PHE	2.8
1	B	218	VAL	2.8
1	B	182	ILE	2.8
1	B	271	LEU	2.7
1	A	237	PHE	2.7
1	B	272	SER	2.7
1	B	296	ASN	2.7
1	B	456	ASN	2.7
1	B	249	THR	2.7
1	B	285	GLU	2.7
1	B	238	ARG	2.6
1	B	245	ASP	2.6
1	B	230	PHE	2.6
1	B	342	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	317	GLY	2.6
1	B	231	PHE	2.6
1	B	215	LYS	2.6
1	A	133	GLN	2.6
1	B	313	GLY	2.6
1	A	248	ILE	2.5
1	B	259	ILE	2.5
1	B	95	TRP	2.5
1	B	312	SER	2.5
1	B	216	GLU	2.5
1	B	282	ASP	2.5
1	B	181	HIS	2.5
1	B	393	SER	2.5
1	A	134	ARG	2.5
1	B	328	ALA	2.4
1	B	135	LEU	2.4
1	B	279	GLU	2.4
1	B	344	ARG	2.4
1	B	223	ASP	2.4
1	B	190	PHE	2.4
1	B	188	ASP	2.3
1	B	207	PHE	2.3
1	B	236	PHE	2.3
1	B	406	PHE	2.3
1	B	226	ILE	2.3
1	B	132	ARG	2.3
1	B	193	CYS	2.3
1	B	391	ASN	2.3
1	B	175	ALA	2.3
1	B	404	TYR	2.3
1	B	141	HIS	2.2
1	B	148	LEU	2.2
1	B	232	GLU	2.2
1	A	284	ILE	2.2
1	B	297	TYR	2.2
1	B	384	PHE	2.2
1	A	41	ARG	2.2
1	A	407	TYR	2.2
1	B	211	LEU	2.2
1	B	244	THR	2.2
1	B	201	HIS	2.2
1	B	335	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	153	ILE	2.1
1	B	222	ALA	2.1
1	B	310	LEU	2.1
1	B	243	CYS	2.1
1	B	339	TRP	2.1
1	B	136	GLU	2.1
1	A	172	PHE	2.0
1	B	291	ASP	2.0
1	B	394	SER	2.0
1	B	173	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 monosaccharides in this entry.

6.4 Ligands [i](#)

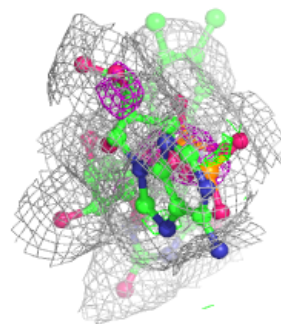
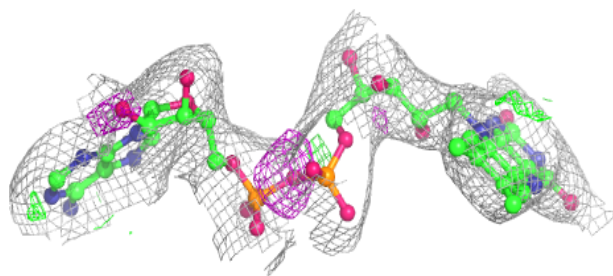
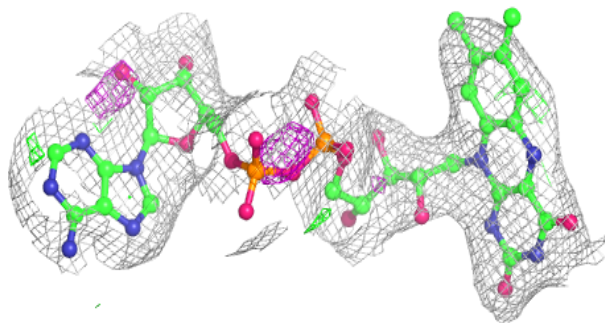
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CIT	B	703	13/13	0.54	0.11	144,145,175,175	0
2	FAD	B	701	53/53	0.78	0.13	102,125,139,142	0
4	CIT	A	703	13/13	0.82	0.09	121,124,150,150	0
2	FAD	A	701	53/53	0.93	0.09	80,88,100,101	0
3	SAH	B	702	26/26	0.96	0.08	60,64,69,70	0
3	SAH	A	702	26/26	0.97	0.07	47,53,59,61	0

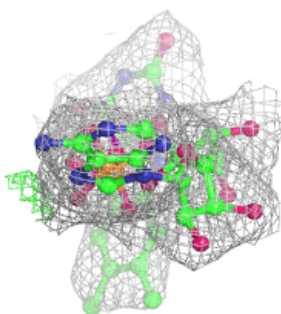
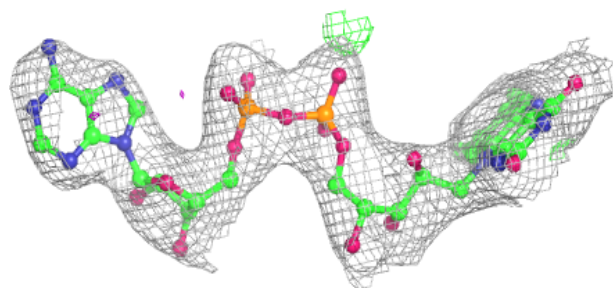
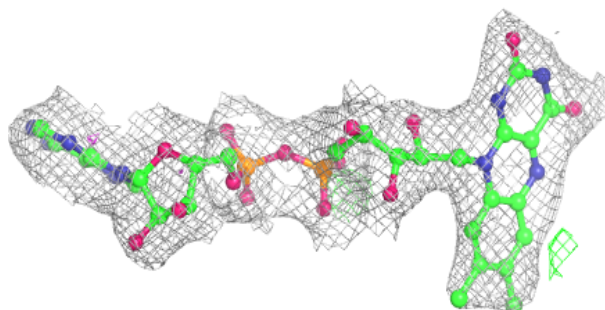
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD 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)

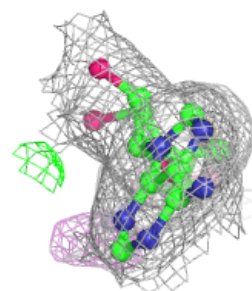
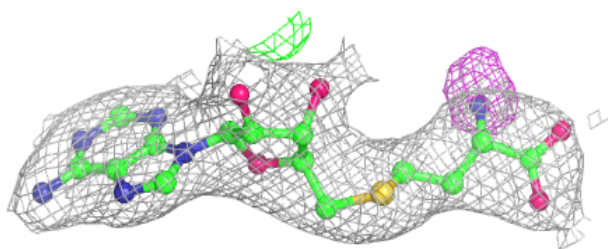
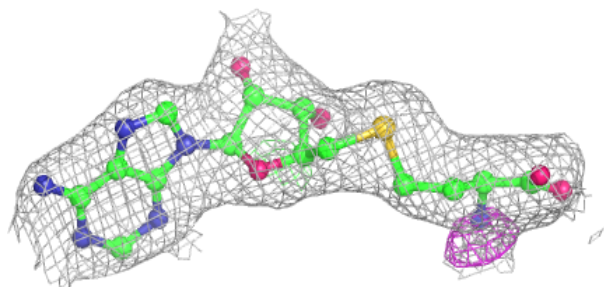
**Electron density around FAD A 701:**

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

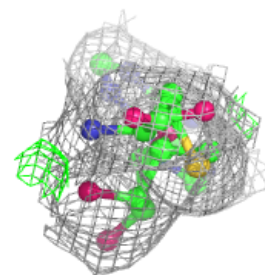
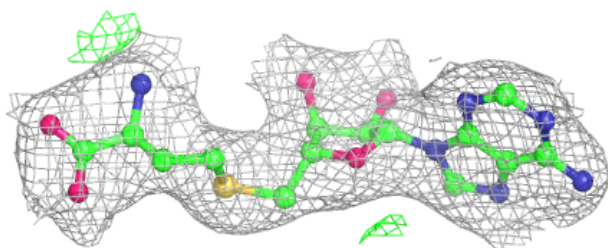
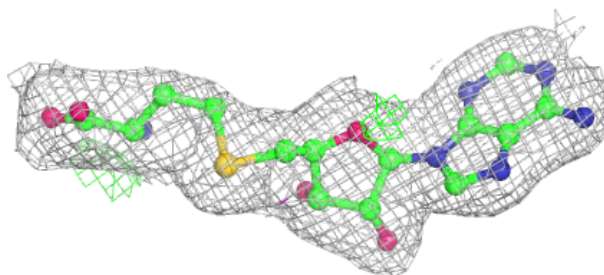


Electron density around SAH B 702:

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

**Electron density around SAH 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.