



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:51 PM UTC

PDB ID : 8W0C / pdb_00008w0c
Title : Crystal structure of Acetyl-CoA synthetase 2 from *Candida albicans* in complex with a cyclopentyl ester AMP inhibitor
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-02-13
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

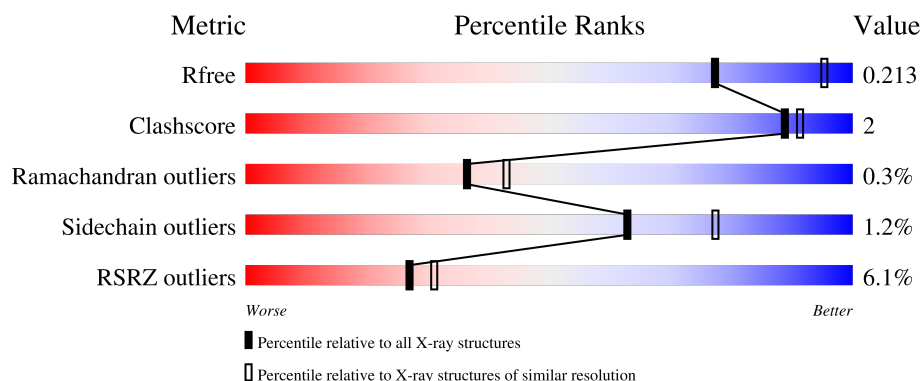
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

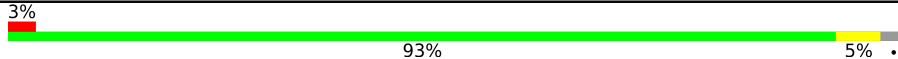
The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	686	
1	B	686	
1	C	686	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14966 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 Acetyl-coenzyme A synthetase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	667	Total	C	N	O	S	0	1	0
			5168	3296	878	980	14			
1	B	642	Total	C	N	O	S	0	0	0
			4973	3178	846	935	14			
1	C	525	Total	C	N	O	S	0	1	0
			4128	2650	694	771	13			

There are 51 discrepancies between the modelled and reference sequences:

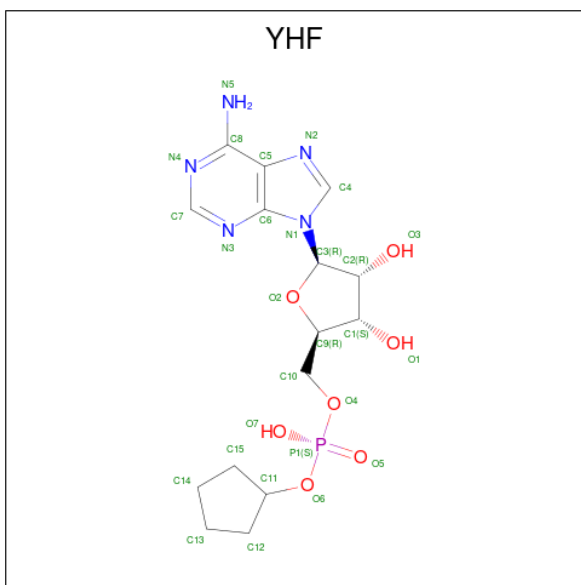
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NJJN3
A	2	HIS	-	expression tag	UNP Q8NJJN3
A	3	HIS	-	expression tag	UNP Q8NJJN3
A	4	HIS	-	expression tag	UNP Q8NJJN3
A	5	HIS	-	expression tag	UNP Q8NJJN3
A	6	HIS	-	expression tag	UNP Q8NJJN3
A	7	HIS	-	expression tag	UNP Q8NJJN3
A	8	HIS	-	expression tag	UNP Q8NJJN3
A	9	HIS	-	expression tag	UNP Q8NJJN3
A	10	GLU	-	expression tag	UNP Q8NJJN3
A	11	ASN	-	expression tag	UNP Q8NJJN3
A	12	LEU	-	expression tag	UNP Q8NJJN3
A	13	TYR	-	expression tag	UNP Q8NJJN3
A	14	PHE	-	expression tag	UNP Q8NJJN3
A	15	GLN	-	expression tag	UNP Q8NJJN3
A	16	GLY	-	expression tag	UNP Q8NJJN3
A	403	ALA	VAL	engineered mutation	UNP Q8NJJN3
B	1	MET	-	initiating methionine	UNP Q8NJJN3
B	2	HIS	-	expression tag	UNP Q8NJJN3
B	3	HIS	-	expression tag	UNP Q8NJJN3
B	4	HIS	-	expression tag	UNP Q8NJJN3
B	5	HIS	-	expression tag	UNP Q8NJJN3
B	6	HIS	-	expression tag	UNP Q8NJJN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8N3N3
B	8	HIS	-	expression tag	UNP Q8N3N3
B	9	HIS	-	expression tag	UNP Q8N3N3
B	10	GLU	-	expression tag	UNP Q8N3N3
B	11	ASN	-	expression tag	UNP Q8N3N3
B	12	LEU	-	expression tag	UNP Q8N3N3
B	13	TYR	-	expression tag	UNP Q8N3N3
B	14	PHE	-	expression tag	UNP Q8N3N3
B	15	GLN	-	expression tag	UNP Q8N3N3
B	16	GLY	-	expression tag	UNP Q8N3N3
B	403	ALA	VAL	engineered mutation	UNP Q8N3N3
C	1	MET	-	initiating methionine	UNP Q8N3N3
C	2	HIS	-	expression tag	UNP Q8N3N3
C	3	HIS	-	expression tag	UNP Q8N3N3
C	4	HIS	-	expression tag	UNP Q8N3N3
C	5	HIS	-	expression tag	UNP Q8N3N3
C	6	HIS	-	expression tag	UNP Q8N3N3
C	7	HIS	-	expression tag	UNP Q8N3N3
C	8	HIS	-	expression tag	UNP Q8N3N3
C	9	HIS	-	expression tag	UNP Q8N3N3
C	10	GLU	-	expression tag	UNP Q8N3N3
C	11	ASN	-	expression tag	UNP Q8N3N3
C	12	LEU	-	expression tag	UNP Q8N3N3
C	13	TYR	-	expression tag	UNP Q8N3N3
C	14	PHE	-	expression tag	UNP Q8N3N3
C	15	GLN	-	expression tag	UNP Q8N3N3
C	16	GLY	-	expression tag	UNP Q8N3N3
C	403	ALA	VAL	engineered mutation	UNP Q8N3N3

- Molecule 2 is 5'-O-[(S)-(cyclopentyloxy)(hydroxy)phosphoryl]adenosine (CCD ID: YHF) (formula: C₁₅H₂₂N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	15	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			28	15	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			28	15	5	7	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	254	Total	O	0	0
			254	254		
7	B	241	Total	O	0	0
			241	241		
7	C	79	Total	O	0	0
			79	79		

- Molecule 1: Acetyl-coenzyme A synthetase 2



ASP
LEU
PRO
LYS
THR
ARG
SER
GLY
LYS
ILE
MET
ARG
ARG
ILE
LEU
ARG
LYS
VAL
SER
SER
ASN
GLU
ALA
ASP
GLN
LEU
GLY
ASP
ILE
SER
THR
LEU
SER
ASN
PRO
GLN
SER
VAL
GLU
GLY
ILE
ILE
SER
ALA
PHE
GLY
ALA
GLN
PHE
GLY
LYS
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.41Å 139.41Å 543.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.58 – 2.35 49.58 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.58-2.35) 100.0 (49.58-2.35)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.34Å)	Xtriage
Refinement program	PHENIX (dev_5233: ???)	Depositor
R, R_{free}	0.181 , 0.210 0.184 , 0.213	Depositor DCC
R_{free} test set	6634 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14966	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: CL, YHF, GOL, NA, SO4

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	0.23	0/5301	0.42	0/7209
1	B	0.22	0/5100	0.42	0/6937
1	C	0.17	0/4250	0.34	0/5787
All	All	0.21	0/14651	0.40	0/19933

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	646	ARG	Sidechain

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	5168	0	5046	12	0
1	B	4973	0	4842	27	0
1	C	4128	0	3991	14	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
5	B	1	0	0	0	0
6	B	6	0	8	1	0
7	A	254	0	0	0	0
7	B	241	0	0	1	0
7	C	79	0	0	0	0
All	All	14966	0	13887	53	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 2.

All (53) 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:675:ILE:HA	1:B:678:ALA:HB3	1.74	0.69
1:B:636:LEU:HD23	1:B:637:PRO:HD2	1.75	0.68
1:B:636:LEU:HD22	1:B:649:LEU:CD2	2.27	0.65
1:B:636:LEU:HD23	1:B:637:PRO:CD	2.29	0.63
1:B:646:ARG:HA	1:B:649:LEU:HD12	1.82	0.62
1:A:493:GLU:OE1	1:A:545:ARG:NH1	2.37	0.58
1:B:479:ILE:HD11	1:B:527:TYR:CG	2.44	0.53
1:B:636:LEU:HD11	1:B:675:ILE:HG12	1.92	0.52
1:A:143:ASP:OD1	1:A:146:ARG:NH2	2.42	0.52
1:B:633:VAL:HG21	1:B:636:LEU:HD12	1.92	0.51
1:C:467:ALA:O	1:C:468:SER:OG	2.28	0.50
1:C:420:ILE:O	1:C:420:ILE:HG23	2.12	0.50
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.93	0.50
1:B:648:ILE:O	1:B:652:VAL:HG23	2.13	0.49
1:B:169:TYR:CZ	1:B:202:ILE:HD11	2.48	0.49
1:B:675:ILE:O	1:B:676:ILE:C	2.58	0.47
1:B:636:LEU:HD22	1:B:649:LEU:HG	1.96	0.47
1:C:522:ASN:N	1:C:523:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG22	1:A:535:ALA:HB1	1.97	0.46
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.51	0.46
1:B:594:TYR:CD2	1:B:649:LEU:HD22	2.52	0.45
1:B:664:SER:HA	1:B:669:PRO:HB3	1.98	0.45
1:C:169:TYR:CZ	1:C:202:ILE:HD11	2.51	0.45
1:C:481:PRO:HG3	1:C:495:VAL:HG23	1.98	0.45
1:A:522:ASN:N	1:A:523:PRO:CD	2.80	0.45
1:A:579:VAL:CG1	1:A:591:VAL:HG13	2.46	0.45
1:B:479:ILE:HD12	1:B:497:ALA:CB	2.46	0.45
1:C:476:ALA:HA	1:C:498:ILE:HD13	1.99	0.44
1:B:420:ILE:O	1:B:420:ILE:HG23	2.17	0.44
1:C:25:VAL:HG22	1:C:535:ALA:HB1	1.98	0.44
1:C:332:PHE:HB2	1:C:358:ILE:HD12	1.99	0.43
1:C:347:LEU:C	1:C:347:LEU:HD23	2.43	0.43
6:B:704:GOL:H32	7:B:996:HOH:O	2.19	0.42
1:B:128:CYS:SG	1:B:174:ALA:HB2	2.60	0.42
1:B:444:TRP:HB3	1:B:451:HIS:HA	2.01	0.42
1:B:594:TYR:CD1	1:B:631:ILE:HB	2.54	0.42
1:A:413:LEU:HB3	1:A:428:TYR:CZ	2.55	0.42
1:B:522:ASN:N	1:B:523:PRO:CD	2.83	0.42
1:B:299:GLY:HA2	1:B:647:ARG:HH11	1.85	0.42
1:C:444:TRP:HB3	1:C:451:HIS:HA	2.01	0.42
1:B:614:VAL:HG13	1:B:626:ALA:HB1	2.02	0.41
1:C:468:SER:OG	1:C:469:TYR:N	2.53	0.41
1:B:635:ASP:O	1:B:675:ILE:HD11	2.21	0.41
1:C:300:THR:HB	1:C:301:PRO:HD2	2.02	0.41
1:A:347:LEU:HD23	1:A:347:LEU:C	2.46	0.41
1:C:413:LEU:HB3	1:C:428:TYR:CZ	2.56	0.41
1:A:444:TRP:HB3	1:A:451:HIS:HA	2.03	0.40
1:C:325:ILE:HD13	1:C:383:HIS:CE1	2.56	0.40
1:A:420:ILE:O	1:A:420:ILE:HG23	2.21	0.40
1:A:658:ASP:O	1:A:659:GLN:CB	2.69	0.40
1:B:636:LEU:HD22	1:B:649:LEU:CG	2.51	0.40
1:B:102:LEU:N	1:B:102:LEU:HD12	2.37	0.40
1:A:169:TYR:CZ	1:A:202:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	666/686 (97%)	647 (97%)	17 (3%)	2 (0%)	36	43
1	B	634/686 (92%)	616 (97%)	16 (2%)	2 (0%)	36	43
1	C	522/686 (76%)	503 (96%)	18 (3%)	1 (0%)	43	52
All	All	1822/2058 (88%)	1766 (97%)	51 (3%)	5 (0%)	36	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	SER
1	B	417	GLY
1	B	468	SER
1	C	468	SER
1	A	417	GLY

5.3.2 Protein sidechains

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	544/568 (96%)	536 (98%)	8 (2%)	57	72
1	B	522/568 (92%)	512 (98%)	10 (2%)	50	65
1	C	433/568 (76%)	433 (100%)	0	100	100
All	All	1499/1704 (88%)	1481 (99%)	18 (1%)	63	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	132	ASP
1	A	177	ILE
1	A	221	LYS
1	A	300	THR
1	A	598	LYS
1	A	616	GLN
1	A	651	LYS
1	B	162	LYS
1	B	221	LYS
1	B	418	GLU
1	B	611	LYS
1	B	636	LEU
1	B	647	ARG
1	B	649	LEU
1	B	653	SER
1	B	654	SER
1	B	677	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	120	ASN
1	A	659	GLN
1	B	46	ASN
1	B	49	HIS
1	B	438	HIS
1	B	655	ASN
1	C	445	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z > 2$
4	SO4	A	703	-	4,4,4	0.72	0	6,6,6	0.34	0
4	SO4	B	705	-	4,4,4	0.66	0	6,6,6	0.09	0
4	SO4	C	703	-	4,4,4	0.75	0	6,6,6	0.30	0
2	YHF	A	701	-	31,31,31	0.42	0	44,46,46	0.60	0
2	YHF	B	701	-	31,31,31	0.41	0	44,46,46	0.57	0
4	SO4	B	706	-	4,4,4	0.76	0	6,6,6	0.13	0
6	GOL	B	704	-	5,5,5	0.42	0	5,5,5	0.49	0
4	SO4	C	702	-	4,4,4	0.68	0	6,6,6	0.13	0
2	YHF	C	701	-	31,31,31	0.41	0	44,46,46	0.59	0
4	SO4	A	704	-	4,4,4	0.81	0	6,6,6	0.25	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	YHF	A	701	-	-	0/15/38/38	0/4/4/4
2	YHF	B	701	-	-	0/15/38/38	0/4/4/4
6	GOL	B	704	-	-	0/4/4/4	-
2	YHF	C	701	-	-	0/15/38/38	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

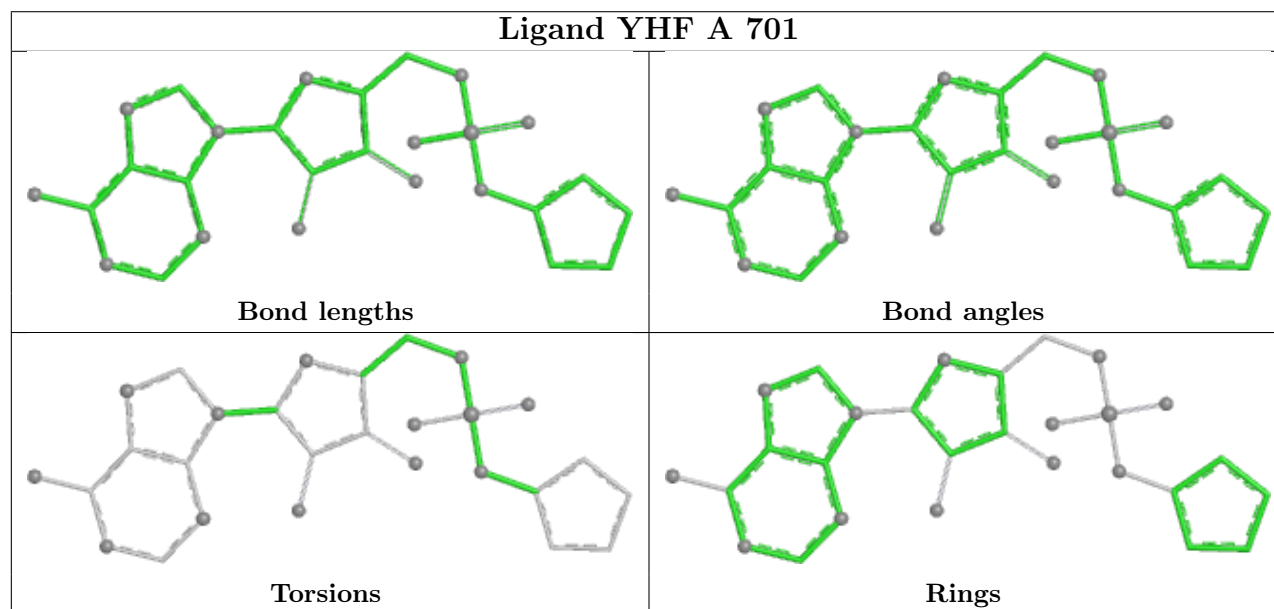
There are no torsion outliers.

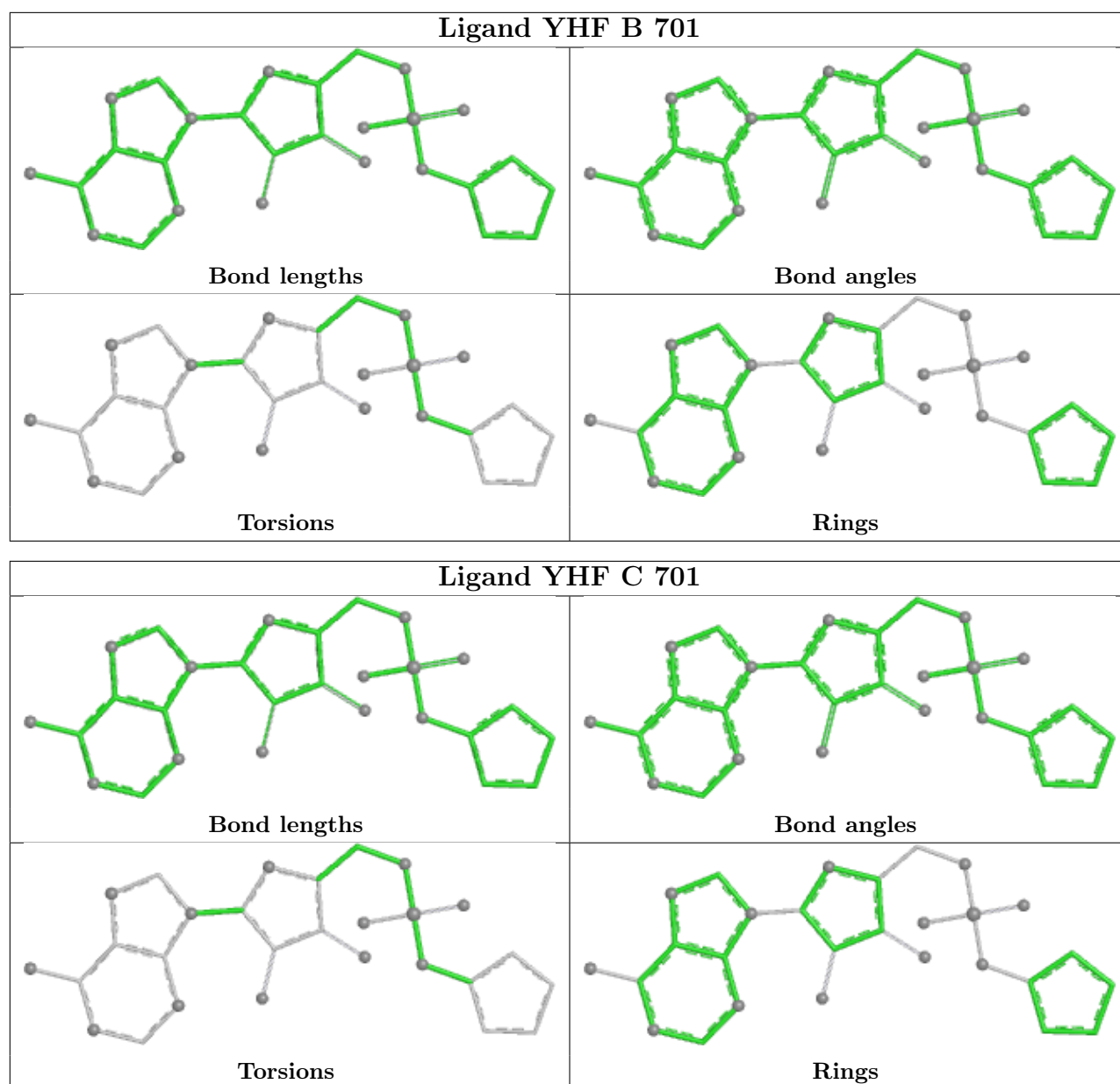
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	704	GOL	1	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	667/686 (97%)	-0.05	24 (3%)	46	52	33, 47, 78, 136	1 (0%)
1	B	642/686 (93%)	0.20	70 (10%)	10	12	35, 47, 121, 197	0
1	C	525/686 (76%)	0.28	18 (3%)	48	55	34, 63, 99, 124	1 (0%)
All	All	1834/2058 (89%)	0.13	112 (6%)	27	31	33, 51, 100, 197	2 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	VAL	6.9
1	B	676	ILE	6.6
1	B	636	LEU	6.2
1	C	549	ASP	6.1
1	B	637	PRO	5.7
1	B	586	ILE	5.0
1	B	683	PHE	4.8
1	B	20	GLN	4.7
1	C	20	GLN	4.7
1	B	665	THR	4.6
1	A	603	ASP	4.6
1	B	644	ILE	4.6
1	B	295	SER	4.5
1	C	300	THR	4.4
1	B	575	SER	4.3
1	B	607	GLU	4.2
1	A	19	GLU	4.1
1	A	298	THR	4.1
1	B	574	VAL	4.0
1	A	601	ASN	4.0
1	A	20	GLN	4.0
1	A	685	LYS	3.9
1	B	633	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	632	ILE	3.8
1	B	655	ASN	3.8
1	A	557	HIS	3.8
1	A	297	SER	3.7
1	A	604	GLU	3.7
1	C	482	VAL	3.7
1	B	577	ALA	3.6
1	B	643	LYS	3.6
1	B	664	SER	3.5
1	A	684	GLY	3.5
1	B	549	ASP	3.5
1	B	645	MET	3.5
1	B	652	VAL	3.4
1	A	602	SER	3.4
1	B	647	ARG	3.4
1	B	420	ILE	3.3
1	B	679	PHE	3.3
1	B	557	HIS	3.2
1	C	54	ASN	3.2
1	A	300	THR	3.2
1	B	640	ARG	3.1
1	B	479	ILE	3.1
1	B	638	LYS	3.1
1	B	654	SER	3.1
1	B	680	GLY	3.0
1	B	572	LYS	3.0
1	B	634	GLN	3.0
1	B	576	GLU	3.0
1	B	546	GLY	3.0
1	B	649	LEU	2.9
1	B	648	ILE	2.9
1	A	599	GLU	2.9
1	B	421	SER	2.9
1	B	677	SER	2.9
1	B	299	GLY	2.8
1	B	642	GLY	2.8
1	B	573	LYS	2.8
1	B	578	ALA	2.8
1	C	225	ARG	2.8
1	B	550	ASP	2.8
1	A	296	GLY	2.7
1	B	682	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	609	LEU	2.7
1	A	47	LYS	2.7
1	B	666	LEU	2.7
1	C	26	HIS	2.7
1	A	619	LYS	2.6
1	B	651	LYS	2.6
1	B	678	ALA	2.6
1	A	605	ASP	2.5
1	B	674	GLY	2.5
1	C	30	GLY	2.5
1	C	294	THR	2.5
1	A	32	LYS	2.5
1	C	51	HIS	2.5
1	B	225	ARG	2.4
1	B	650	ARG	2.4
1	A	624	PHE	2.4
1	C	420	ILE	2.4
1	B	21	THR	2.4
1	B	585	ASP	2.3
1	C	419	PRO	2.3
1	C	21	THR	2.3
1	C	36	THR	2.3
1	B	646	ARG	2.3
1	B	595	VAL	2.3
1	A	572	LYS	2.3
1	B	641	SER	2.3
1	C	302	LYS	2.3
1	B	580	VAL	2.2
1	C	489	GLY	2.2
1	B	639	THR	2.2
1	B	681	ALA	2.2
1	B	671	SER	2.2
1	B	631	ILE	2.2
1	A	635	ASP	2.2
1	B	32	LYS	2.2
1	B	26	HIS	2.2
1	B	569	ILE	2.1
1	B	673	GLU	2.1
1	B	588	GLY	2.1
1	B	589	GLN	2.1
1	C	38	LYS	2.1
1	B	294	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	612	GLU	2.0
1	A	553	ASN	2.0
1	C	368	ASP	2.0
1	A	586	ILE	2.0
1	B	675	ILE	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](#)

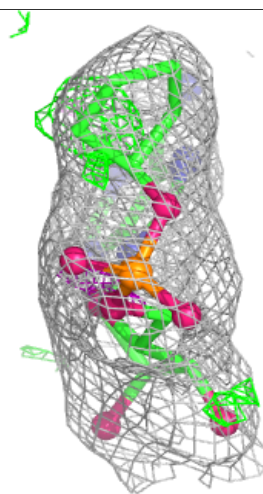
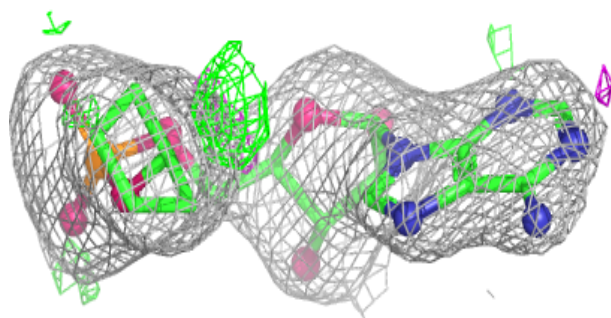
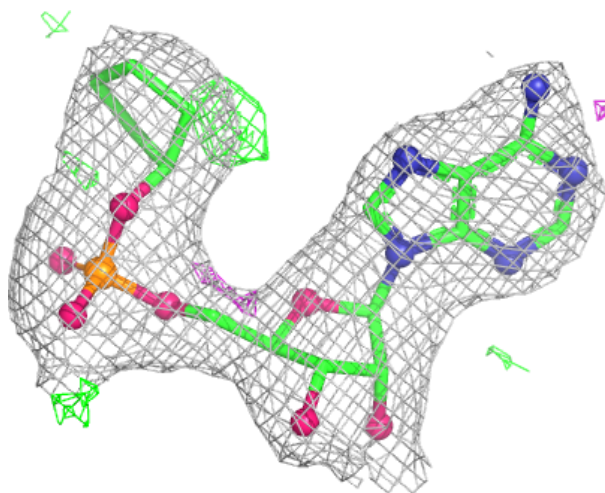
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	B	704	6/6	0.53	0.24	58,62,65,67	0
4	SO4	A	704	5/5	0.74	0.15	61,64,89,100	0
4	SO4	B	706	5/5	0.77	0.18	55,69,95,97	0
4	SO4	C	702	5/5	0.79	0.11	98,100,106,122	0
4	SO4	A	703	5/5	0.82	0.12	67,75,84,85	0
4	SO4	B	705	5/5	0.83	0.15	91,93,104,112	0
4	SO4	C	703	5/5	0.86	0.15	70,72,84,104	0
2	YHF	C	701	28/28	0.92	0.11	65,72,80,83	0
5	CL	B	703	1/1	0.97	0.22	80,80,80,80	0
2	YHF	B	701	28/28	0.97	0.06	42,47,51,54	0
3	NA	A	702	1/1	0.98	0.05	42,42,42,42	0
3	NA	B	702	1/1	0.98	0.03	44,44,44,44	0
2	YHF	A	701	28/28	0.99	0.05	33,39,45,47	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.

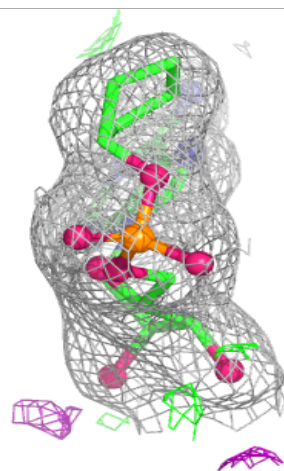
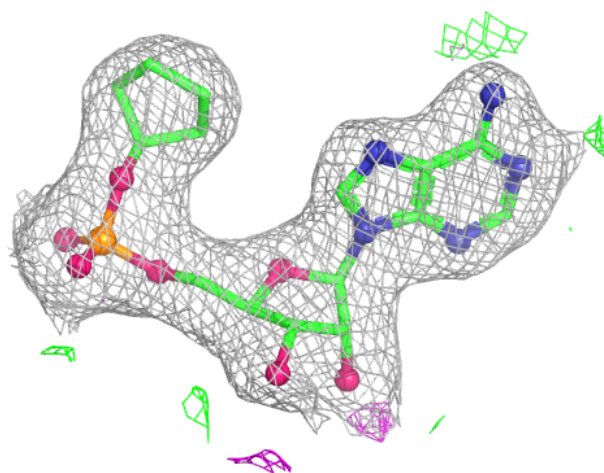
Electron density around YHF C 701:

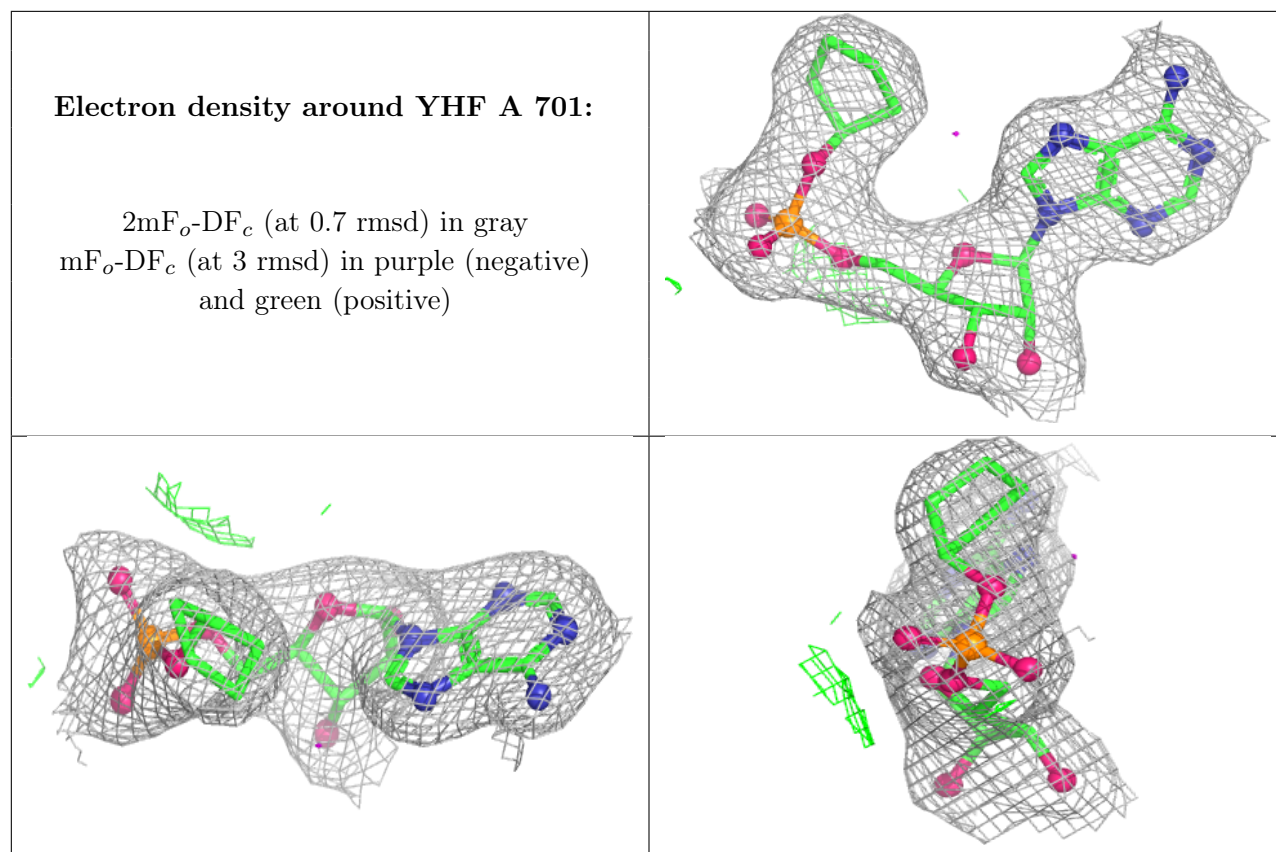
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around YHF 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.