



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:20 AM UTC

PDB ID : 5VPV / pdb_00005vpv
Title : Crystal structure of Apo Cryptococcus neoformans H99 Acetyl-CoA Synthetase with an Acetylated Active Site Lysine
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID); Fox III, D.; Davies, D.R.; Calhoun, B.
Deposited on : 2017-05-05
Resolution : 2.60 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
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

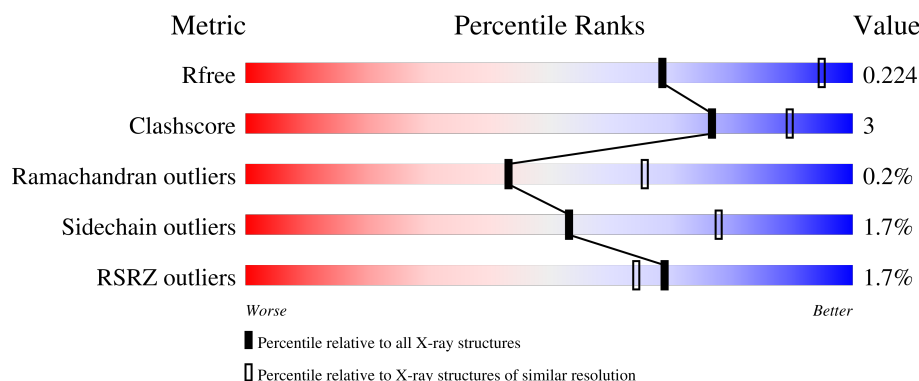
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	694	% 86% 8% 5%
1	B	694	3% 85% 7% 6%
1	C	694	68% 6% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14915 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	657	Total	C	N	O	S	0	2	0
			5111	3264	870	951	26			
1	B	649	Total	C	N	O	S	0	3	0
			4971	3175	854	916	26			
1	C	519	Total	C	N	O	S	0	2	0
			4085	2614	694	754	23			

There are 45 discrepancies between the modelled and reference sequences:

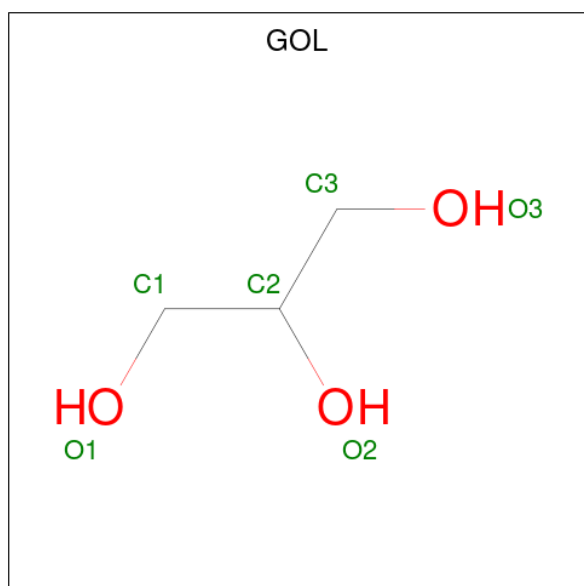
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression tag	UNP J9VFT1
A	-6	HIS	-	expression tag	UNP J9VFT1
A	-5	HIS	-	expression tag	UNP J9VFT1
A	-4	GLU	-	expression tag	UNP J9VFT1
A	-3	ASN	-	expression tag	UNP J9VFT1
A	-2	LEU	-	expression tag	UNP J9VFT1
A	-1	TYR	-	expression tag	UNP J9VFT1
A	0	PHE	-	expression tag	UNP J9VFT1
A	1	GLN	-	expression tag	UNP J9VFT1
B	-13	MET	-	initiating methionine	UNP J9VFT1
B	-12	HIS	-	expression tag	UNP J9VFT1
B	-11	HIS	-	expression tag	UNP J9VFT1
B	-10	HIS	-	expression tag	UNP J9VFT1
B	-9	HIS	-	expression tag	UNP J9VFT1
B	-8	HIS	-	expression tag	UNP J9VFT1
B	-7	HIS	-	expression tag	UNP J9VFT1
B	-6	HIS	-	expression tag	UNP J9VFT1

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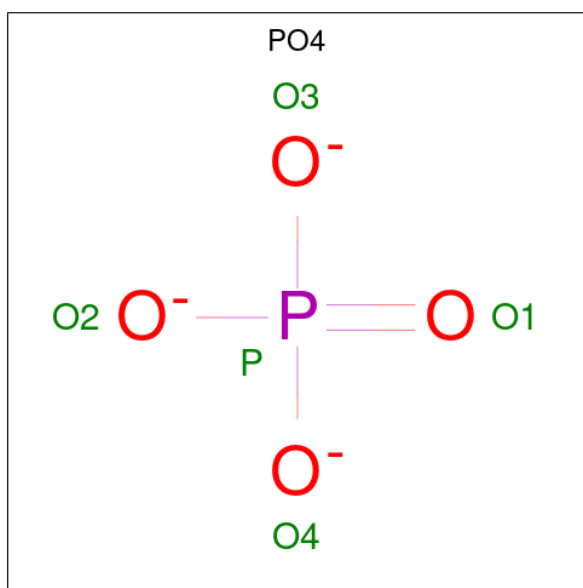
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
C	-13	MET	-	initiating methionine	UNP J9VFT1
C	-12	HIS	-	expression tag	UNP J9VFT1
C	-11	HIS	-	expression tag	UNP J9VFT1
C	-10	HIS	-	expression tag	UNP J9VFT1
C	-9	HIS	-	expression tag	UNP J9VFT1
C	-8	HIS	-	expression tag	UNP J9VFT1
C	-7	HIS	-	expression tag	UNP J9VFT1
C	-6	HIS	-	expression tag	UNP J9VFT1
C	-5	HIS	-	expression tag	UNP J9VFT1
C	-4	GLU	-	expression tag	UNP J9VFT1
C	-3	ASN	-	expression tag	UNP J9VFT1
C	-2	LEU	-	expression tag	UNP J9VFT1
C	-1	TYR	-	expression tag	UNP J9VFT1
C	0	PHE	-	expression tag	UNP J9VFT1
C	1	GLN	-	expression tag	UNP J9VFT1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

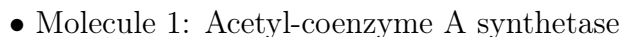
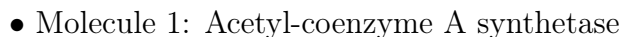


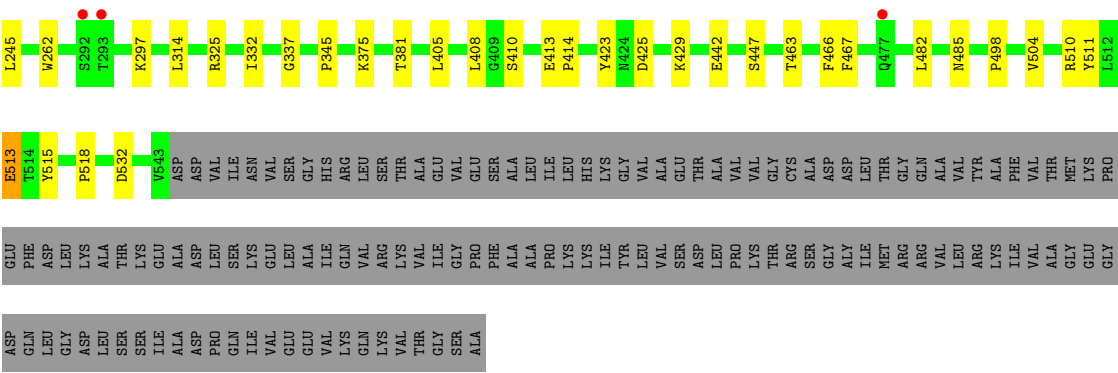
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total 276	O 276	0	1
4	B	220	Total 220	O 220	0	0
4	C	188	Total 189	O 189	0	1

- Molecule 1: Acetyl-coenzyme A synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.98Å 176.98Å 159.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.60 49.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.28-2.60) 100.0 (49.28-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_2744	Depositor
R, R_{free}	0.156 , 0.216 (Not available) , 0.224	Depositor DCC
R_{free} test set	3905 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14915	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: GOL, ALY, PO4

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	0.30	0/5237	0.50	0/7132
1	B	0.30	0/5112	0.50	0/6969
1	C	0.31	0/4214	0.51	0/5743
All	All	0.30	0/14563	0.50	0/19844

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	60	GLY	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	5111	0	4931	28	0
1	B	4971	0	4710	27	0
1	C	4085	0	3910	25	0
2	A	24	0	32	1	0
2	B	12	0	16	0	0
2	C	12	0	16	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	276	0	0	1	0
4	B	220	0	0	2	0
4	C	189	0	0	0	0
All	All	14915	0	13615	80	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 3.

All (80) 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:592:MET:HE3	1:B:606:LEU:HD21	1.57	0.87
1:A:634:PRO:HB2	1:A:642:MET:HE3	1.68	0.74
1:C:134:GLU:OE2	1:C:325[A]:ARG:NH2	2.36	0.59
1:C:314:LEU:HD22	1:C:345:PRO:HA	1.83	0.59
1:B:254:MET:HE2	1:B:261:TRP:CE2	2.39	0.57
1:C:405:LEU:HD13	1:C:408:LEU:HD21	1.89	0.54
1:B:504:VAL:HG23	1:B:511:TYR:HB2	1.88	0.54
1:B:152:LYS:NZ	4:B:805:HOH:O	2.41	0.53
1:C:297:LYS:HD3	1:C:510:ARG:NH1	2.23	0.53
1:A:90:GLU:HG2	1:A:91:HIS:CD2	2.45	0.52
1:A:636:THR:HG22	1:A:667:ILE:HG21	1.91	0.52
1:B:442:GLU:HG2	1:B:515:TYR:CZ	2.43	0.52
1:B:431:GLN:OE1	4:B:801:HOH:O	2.18	0.52
1:A:574:VAL:HG13	1:A:586:VAL:HG13	1.94	0.50
1:B:96:TRP:CD1	1:B:498:PRO:HA	2.47	0.50
1:A:495:ARG:NE	4:A:802:HOH:O	2.30	0.50
1:A:209:VAL:HG22	1:A:241:ASN:HB2	1.93	0.49
1:C:72:ARG:HH22	2:C:702:GOL:C3	2.26	0.48
1:A:492:VAL:HB	1:A:522:TYR:HB3	1.96	0.48
1:A:504:VAL:HG23	1:A:511:TYR:HB2	1.96	0.47
1:C:314:LEU:O	1:C:314:LEU:HG	2.14	0.47
1:A:58:THR:HG22	1:A:66:TRP:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:MET:HE2	1:A:261:TRP:CE2	2.49	0.47
1:C:214:ASP:OD1	1:C:215:GLU:N	2.47	0.47
1:B:492:VAL:HB	1:B:522:TYR:HB3	1.96	0.47
1:B:373:LYS:HE2	1:B:374:TRP:CZ2	2.50	0.46
1:C:332:ILE:HA	1:C:337:GLY:HA3	1.97	0.46
1:B:123:ILE:HD11	1:B:325[B]:ARG:HG2	1.98	0.46
1:A:485:ASN:HB3	1:A:532:ASP:O	2.16	0.46
1:A:577:CYS:HB3	1:A:587:TYR:CE1	2.52	0.45
1:B:540:LYS:HG2	1:B:541:GLY:O	2.17	0.45
1:A:442:GLU:HG2	1:A:515:TYR:CZ	2.52	0.45
1:C:58:THR:HG22	1:C:66:TRP:CD2	2.51	0.45
1:C:67:TRP:CZ3	1:C:498:PRO:HG2	2.52	0.45
1:C:72:ARG:HH22	2:C:702:GOL:H31	1.82	0.45
1:B:122:ILE:HA	1:B:352:THR:O	2.16	0.45
1:C:425:ASP:O	1:C:429:LYS:HA	2.16	0.44
1:B:325[B]:ARG:HG3	1:B:351:THR:HB	1.99	0.44
1:C:381:THR:O	1:C:410:SER:HA	2.18	0.44
1:C:442:GLU:HG2	1:C:515:TYR:CZ	2.52	0.44
1:B:314:LEU:HD22	1:B:345:PRO:HA	1.99	0.44
1:A:213:THR:HG22	1:A:245:LEU:HB3	2.00	0.44
1:B:463:THR:OG1	1:B:464:PHE:N	2.51	0.44
1:A:167:PRO:CB	2:A:701:GOL:H31	2.47	0.43
1:A:425:ASP:O	1:A:429:LYS:HA	2.18	0.43
1:C:325[B]:ARG:NH2	1:C:375:LYS:O	2.51	0.43
1:B:109:LEU:HD13	1:B:141:MET:HA	2.01	0.43
1:C:485:ASN:HB3	1:C:532:ASP:O	2.18	0.43
1:A:632:ASP:OD1	1:A:633:LEU:N	2.51	0.43
1:B:475:ASP:HB2	1:B:482:LEU:HD21	2.00	0.43
1:B:524:PHE:CZ	1:B:526:GLY:HA2	2.53	0.43
1:A:26:LEU:HB3	1:A:456:SER:HB3	2.01	0.43
1:A:332:ILE:HA	1:A:337:GLY:HA3	2.00	0.43
1:A:463:THR:OG1	1:A:464:PHE:N	2.47	0.43
1:B:572:THR:HG22	1:B:590:VAL:HG13	2.00	0.43
1:C:243:LEU:HD11	1:C:262:TRP:HA	2.01	0.43
1:A:314:LEU:HD22	1:A:345:PRO:HA	2.01	0.42
1:B:218:ARG:CZ	1:B:358:THR:HG22	2.49	0.42
1:C:413:GLU:HG3	1:C:414:PRO:HD2	2.01	0.42
1:C:466:PHE:CG	1:C:467:PHE:N	2.86	0.42
1:A:566:HIS:HB3	1:A:569:VAL:HG23	2.01	0.42
1:A:632:ASP:HB3	1:A:672:ILE:HD13	2.02	0.42
1:B:288:TYR:HA	1:B:297:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:HD13	1:C:345:PRO:HG3	2.00	0.42
1:C:66:TRP:CH2	1:C:70:LYS:HG3	2.54	0.42
1:B:635:LYS:HA	1:B:640:ALY:O	2.20	0.42
1:B:440:MET:CE	1:B:442:GLU:HB2	2.50	0.42
1:B:586:VAL:HB	1:B:624:PRO:HA	2.01	0.42
1:C:504:VAL:HG23	1:C:511:TYR:HB2	2.02	0.41
1:A:60:GLY:H	1:A:495:ARG:NH1	2.18	0.41
1:B:537:MET:HB2	1:B:537:MET:HE2	1.57	0.41
1:A:233:LEU:HA	1:A:236:CYS:HB2	2.01	0.41
1:C:513:GLU:O	1:C:518:PRO:HD3	2.20	0.41
1:A:509:LYS:HB2	1:A:509:LYS:HE3	1.85	0.41
1:A:408:LEU:HB3	1:A:423:TYR:CZ	2.56	0.40
1:A:635:LYS:N	1:A:642:MET:HE2	2.36	0.40
1:B:413:GLU:HB2	1:B:414:PRO:HD2	2.02	0.40
1:C:213:THR:HG22	1:C:245:LEU:HB3	2.03	0.40
1:C:29:PRO:HA	1:C:30:PRO:HD3	1.96	0.40
1:B:513:GLU:HA	1:B:517:LYS:HG3	2.03	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	650/694 (94%)	620 (95%)	30 (5%)	0	100	100
1	B	641/694 (92%)	619 (97%)	19 (3%)	3 (0%)	24	46
1	C	519/694 (75%)	499 (96%)	19 (4%)	1 (0%)	43	66
All	All	1810/2082 (87%)	1738 (96%)	68 (4%)	4 (0%)	43	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	THR
1	C	463	THR
1	B	631	SER
1	B	61	PRO

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	526/575 (92%)	515 (98%)	11 (2%)	47	73
1	B	497/575 (86%)	488 (98%)	9 (2%)	51	76
1	C	420/575 (73%)	415 (99%)	5 (1%)	63	83
All	All	1443/1725 (84%)	1418 (98%)	25 (2%)	53	78

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

Mol	Chain	Res	Type
1	A	23	SER
1	A	49	GLU
1	A	116	ASN
1	A	373	LYS
1	A	436	ASP
1	A	440	MET
1	A	472	ASP
1	A	473	ILE
1	A	509	LYS
1	A	574	VAL
1	A	655	ASP
1	B	218	ARG
1	B	251	LYS
1	B	297	LYS
1	B	413	GLU
1	B	423	TYR
1	B	483	GLU
1	B	537	MET
1	B	595	GLU

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Mol	Chain	Res	Type
1	B	631	SER
1	C	25	ASP
1	C	423	TYR
1	C	447	SER
1	C	482	LEU
1	C	513	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	613	GLN
1	B	431	GLN
1	B	485	ASN
1	B	552	HIS
1	C	116	ASN
1	C	227	GLN
1	C	241	ASN
1	C	321	HIS
1	C	485	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	ALY	B	640	1	3,4,12	0.72	0	2,4,14	0.63	0
1	ALY	A	640	1	10,11,12	0.91	0	7,12,14	0.88	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
1	ALY	B	640	1	-	1/1/2/12	-
1	ALY	A	640	1	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	640	ALY	O-C-CA-CB
1	A	640	ALY	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	640	ALY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	GOL	A	701	-	5,5,5	1.13	0	5,5,5	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	701	-	5,5,5	1.22	0	5,5,5	0.79	0
3	PO4	C	703	-	4,4,4	0.85	0	6,6,6	0.58	0
3	PO4	B	703	-	4,4,4	0.96	0	6,6,6	0.70	0
2	GOL	B	702	-	5,5,5	0.93	0	5,5,5	1.02	0
2	GOL	A	702	-	5,5,5	1.15	0	5,5,5	0.91	0
2	GOL	A	703	-	5,5,5	0.96	0	5,5,5	1.06	0
2	GOL	A	704	-	5,5,5	1.35	0	5,5,5	0.90	0
2	GOL	B	701	-	5,5,5	0.93	0	5,5,5	1.06	0
3	PO4	A	705	-	4,4,4	0.86	0	6,6,6	0.51	0
2	GOL	C	702	-	5,5,5	0.76	0	5,5,5	1.23	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	GOL	A	701	-	-	4/4/4/4	-
2	GOL	C	701	-	-	2/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-
2	GOL	A	702	-	-	0/4/4/4	-
2	GOL	A	703	-	-	4/4/4/4	-
2	GOL	A	704	-	-	2/4/4/4	-
2	GOL	B	701	-	-	1/4/4/4	-
2	GOL	C	702	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O1-C1-C2-C3
2	A	701	GOL	C1-C2-C3-O3
2	A	703	GOL	O1-C1-C2-C3
2	A	703	GOL	C1-C2-C3-O3
2	B	702	GOL	C1-C2-C3-O3
2	A	701	GOL	O1-C1-C2-O2
2	A	703	GOL	O1-C1-C2-O2
2	A	703	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O2-C2-C3-O3
2	B	701	GOL	O1-C1-C2-O2
2	A	704	GOL	O1-C1-C2-O2
2	A	704	GOL	O2-C2-C3-O3
2	C	701	GOL	O1-C1-C2-C3
2	B	702	GOL	O2-C2-C3-O3
2	C	701	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GOL	1	0
2	C	702	GOL	2	0

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	656/694 (94%)	-0.68	7 (1%) 78 74	17, 30, 66, 102	2 (0%)
1	B	648/694 (93%)	-0.44	21 (3%) 50 44	13, 31, 85, 119	3 (0%)
1	C	519/694 (74%)	-0.70	3 (0%) 85 83	17, 32, 57, 83	2 (0%)
All	All	1823/2082 (87%)	-0.60	31 (1%) 69 64	13, 31, 74, 119	7 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	597	ASP	5.9
1	A	666	SER	5.6
1	A	659	ASP	5.5
1	B	632	ASP	5.2
1	A	294	GLY	4.5
1	A	597	ASP	4.3
1	B	639	GLY	3.9
1	B	605	ASP	3.7
1	B	596	PHE	3.4
1	B	670	PRO	3.1
1	B	296	PRO	3.0
1	B	563	LEU	3.0
1	C	292	SER	2.8
1	B	62	ASN	2.8
1	A	667	ILE	2.7
1	B	25	ASP	2.6
1	C	293	THR	2.5
1	A	602	LYS	2.5
1	B	567	LYS	2.5
1	B	8	PRO	2.5
1	A	681	THR	2.4
1	B	594	PRO	2.4
1	B	24	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	678	GLN	2.3
1	C	477	GLN	2.3
1	B	672	ILE	2.2
1	B	566	HIS	2.2
1	B	21	PRO	2.2
1	B	569	VAL	2.2
1	B	587	TYR	2.2
1	B	414	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	ALY	B	640	5/13	0.67	0.17	75,79,82,88	0
1	ALY	A	640	12/13	0.96	0.08	27,41,49,55	0

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
2	GOL	C	701	6/6	0.70	0.20	69,71,74,78	0
2	GOL	A	704	6/6	0.76	0.20	67,73,79,84	0
2	GOL	B	701	6/6	0.78	0.16	70,82,84,85	0
2	GOL	A	702	6/6	0.82	0.22	52,67,75,75	0
2	GOL	A	703	6/6	0.83	0.14	62,74,77,80	0
2	GOL	B	702	6/6	0.86	0.18	78,85,87,88	0
2	GOL	C	702	6/6	0.87	0.16	61,63,68,73	0
3	PO4	B	703	5/5	0.90	0.26	80,83,90,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	C	703	5/5	0.90	0.18	82,86,88,93	0
3	PO4	A	705	5/5	0.92	0.16	57,61,73,81	0
2	GOL	A	701	6/6	0.96	0.10	46,51,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.