Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:58 pm BST

PDB ID	:	5VPV
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 following versions of software and data (see references ⓘ) were used in the production of this report:

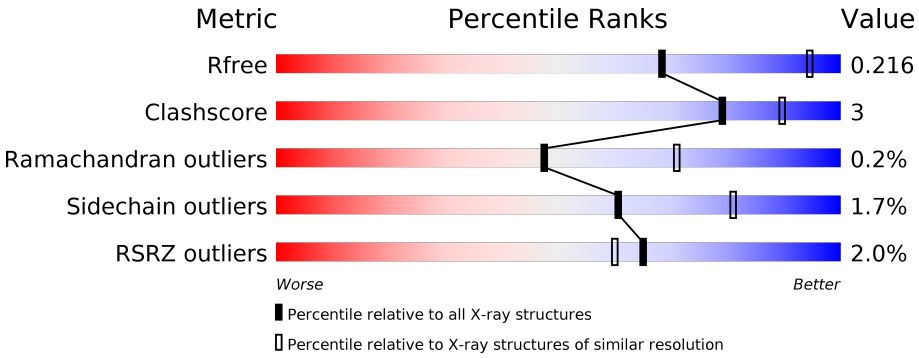
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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 <=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	% 87% 8% 5%
1	B	694	3% 85% 8% 6%
1	C	694	% 68% 6% 25%

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
2	GOL	A	702	-	-	-	X
2	GOL	B	702	-	-	-	X

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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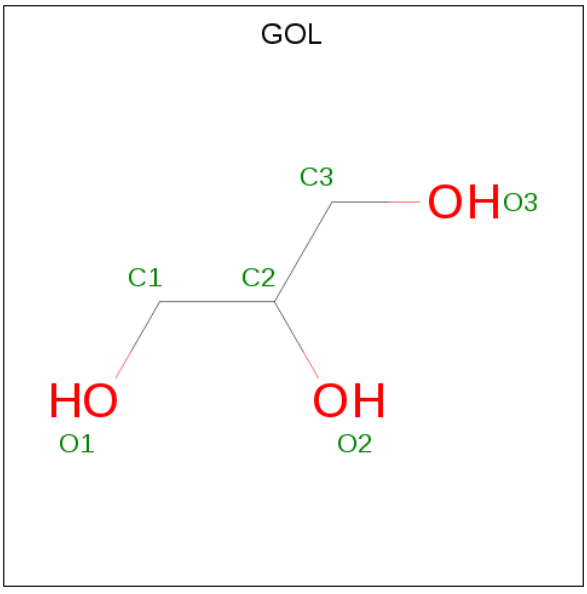
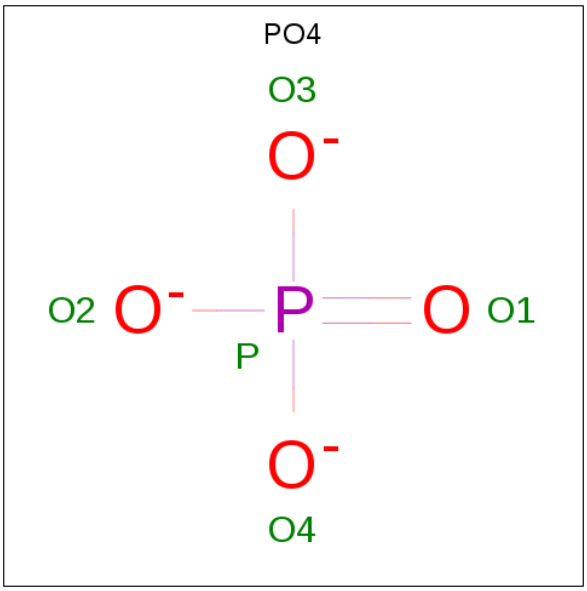
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
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 (three-letter code: 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 (three-letter code: 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.

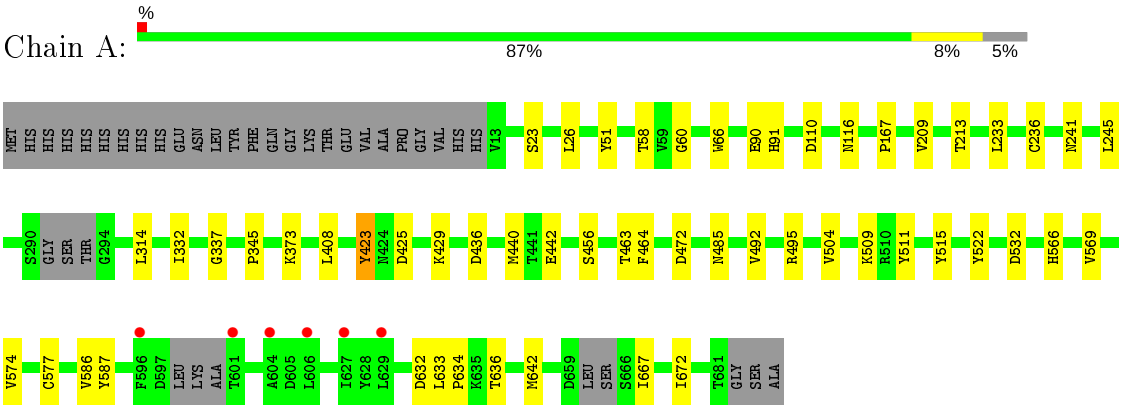
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	275	Total O 276 276	0	1
4	B	220	Total O 220 220	0	0
4	C	188	Total O 189 189	0	1

3 Residue-property plots (i)

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.

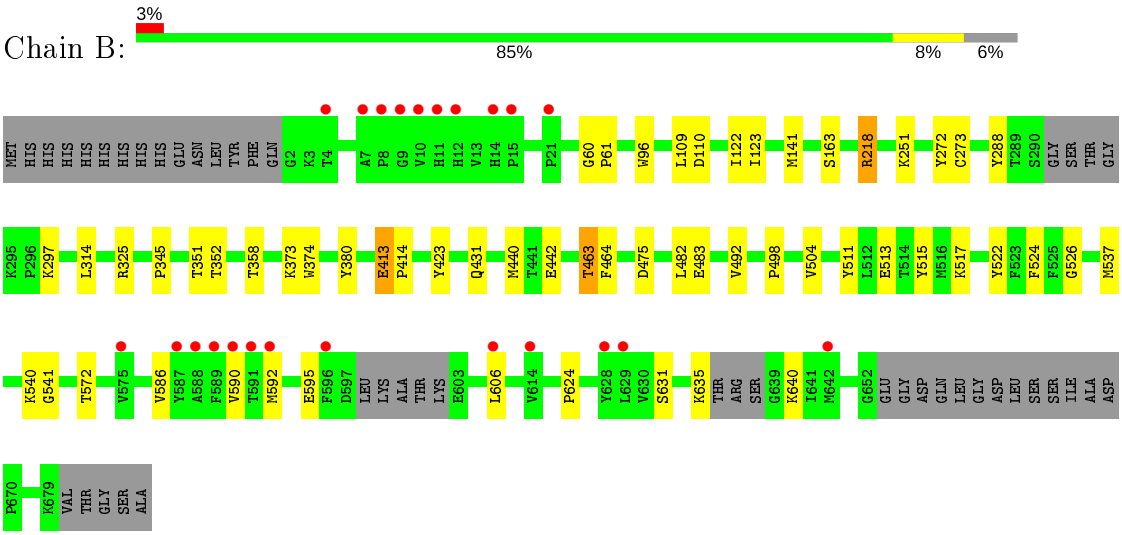
- Molecule 1: Acetyl-coenzyme A synthetase

Chain A:



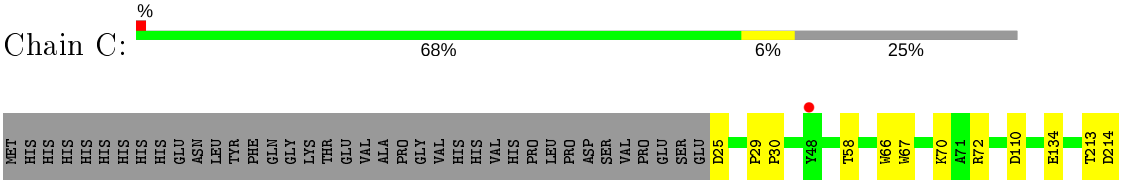
- Molecule 1: Acetyl-coenzyme A synthetase

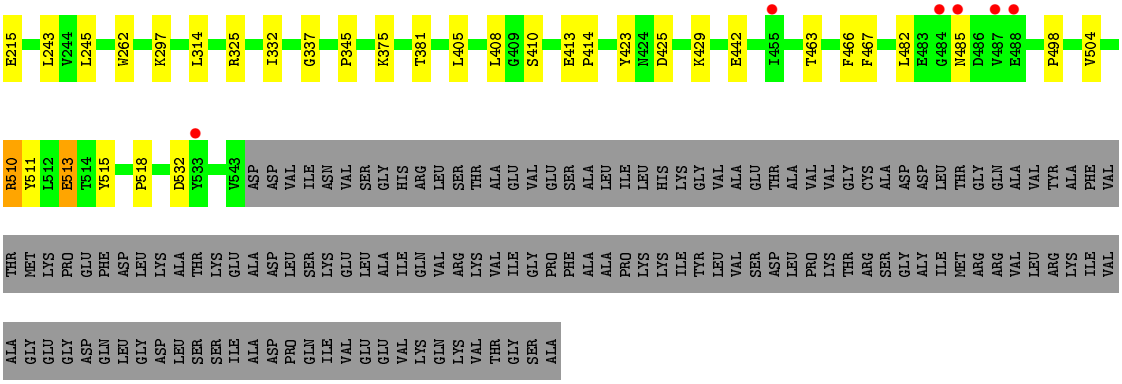
Chain B:



- Molecule 1: Acetyl-coenzyme A synthetase

Chain C:




E215 L243 V244 L245 W262 K297 L314 R325 I332 G337 P345 K375 T381 L405 L408 G409 S410 E413 P414 Y423 N424 D425 K429 E442 I455 T463 F466 F467 L482 E483 G484 N485 D486 V487 E488 P498 V504
R510 Y511 L512 E513 T514 Y515 P518 D532 Y533 V543 ASP ASP VAL ILE ASN VAL SER GLY HIS ARG LEU SER THR ALA GLU VAL GLU SER ALA LEU ILE LEU HIS LYS GLY VAL ALA GLU THR ALA VAL VAL GLY CYS ALA ASP ASP LEU THR GLY GLN ALA VAL TYR ALA PHE VAL
THR MET LYS PRO GLU PHE ASP LEU LYS ALA THR LYS GLU ALA ASP LEU SER LYS GLU LEU ALA ILE GLN VAL ARG LYS VAL ILE GLY PRO PHE ALA ALA PRO LYS LYS ILE TYR LEU VAL SER ASP LEU PRO LYS THR ARG SER GLY ALY ILE MET ARG ARG VAL LEU ARG LYS ILE VAL
ALA GLY GLU GLY ASP GLN LEU GLY ASP LEU SER SER ILE ALA ASP PRO GLN ILE VAL GLU GLU VAL LYS GLN LYS VAL THR GLY SER ALA

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	4.70 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_2744	Depositor
R, R_{free}	0.156 , 0.216 0.156 , 0.216	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 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PO4, ALY

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	0.38	0/5237	0.54	0/7132
1	B	0.38	0/5112	0.54	0/6969
1	C	0.39	0/4214	0.56	0/5743
All	All	0.38	0/14563	0.54	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

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	27	0
1	B	4971	0	4709	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	1	0
4	C	189	0	0	0	0
All	All	14915	0	13614	79	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 (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C: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:A:634:PRO:HB2	1:A:642:MET:HE2	1.85	0.59
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:C:297:LYS:HD3	1:C:510:ARG:NH1	2.23	0.53
1:A:636:THR:HG22	1:A:667:ILE:HG21	1.91	0.52
1:A:90:GLU:HG2	1:A:91:HIS:CD2	2.45	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:B:592:MET:HE3	1:B:606:LEU:HD21	1.95	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:HG	1:C:314:LEU:O	2.14	0.47
1:A:58:THR:HG22	1:A:66:TRP:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:463:THR:OG1	1:A:464:PHE:N	2.47	0.45
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:B:592:MET:CE	1:B:606:LEU:HD21	2.49	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: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:314:LEU:O	1:A:314:LEU:HG	2.19	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
1:C:314:LEU:HD13	1:C:345:PRO:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:272:TYR:CG	1:B:273:CYS:N	2.89	0.41
1:A:408:LEU:HB3	1:A:423:TYR:CZ	2.56	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:440:MET:HE2	1:B:440:MET:HB2	1.90	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 (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	650/694 (94%)	620 (95%)	30 (5%)	0	100	100
1	B	641/694 (92%)	619 (97%)	19 (3%)	3 (0%)	29	52
1	C	519/694 (75%)	499 (96%)	19 (4%)	1 (0%)	47	71
All	All	1810/2082 (87%)	1738 (96%)	68 (4%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	THR

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

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	526/575 (92%)	517 (98%)	9 (2%)	60	81
1	B	497/575 (86%)	487 (98%)	10 (2%)	55	78
1	C	420/575 (73%)	414 (99%)	6 (1%)	67	85
All	All	1443/1725 (84%)	1418 (98%)	25 (2%)	60	81

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

Mol	Chain	Res	Type
1	A	23	SER
1	A	51	TYR
1	A	110	ASP
1	A	116	ASN
1	A	373	LYS
1	A	423	TYR
1	A	436	ASP
1	A	440	MET
1	A	472	ASP
1	B	110	ASP
1	B	163	SER
1	B	218	ARG
1	B	251	LYS
1	B	380	TYR
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	C	25	ASP
1	C	110	ASP
1	C	423	TYR
1	C	482	LEU
1	C	510	ARG
1	C	513	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	613	GLN
1	B	431	GLN
1	C	116	ASN
1	C	321	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.69	0	2,4,14	0.66	0
1	ALY	A	640	1	10,11,12	0.87	0	7,12,14	0.92	1 (14%)

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	-	0/0/2/12	-
1	ALY	A	640	1	-	1/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	640	ALY	CD-CG-CB	-2.12	106.12	113.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 carbohydrates 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	$\#\|Z\| > 2$
3	PO4	A	705	-	4,4,4	0.81	0	6,6,6	0.48	0
2	GOL	B	702	-	5,5,5	0.90	0	5,5,5	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	A	704	-	5,5,5	1.27	0	5,5,5	0.84	0
2	GOL	B	701	-	5,5,5	0.90	0	5,5,5	0.98	0
3	PO4	B	703	-	4,4,4	0.92	0	6,6,6	0.66	0
2	GOL	C	701	-	5,5,5	1.16	0	5,5,5	0.74	0
2	GOL	A	701	-	5,5,5	1.08	0	5,5,5	0.87	0
3	PO4	C	703	-	4,4,4	0.81	0	6,6,6	0.55	0
2	GOL	A	702	-	5,5,5	1.10	0	5,5,5	0.84	0
2	GOL	C	702	-	5,5,5	0.75	0	5,5,5	1.14	0
2	GOL	A	703	-	5,5,5	0.92	0	5,5,5	0.98	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	B	702	-	-	2/4/4/4	-
2	GOL	A	704	-	-	3/4/4/4	-
2	GOL	B	701	-	-	2/4/4/4	-
2	GOL	C	701	-	-	2/4/4/4	-
2	GOL	A	701	-	-	4/4/4/4	-
2	GOL	A	702	-	-	0/4/4/4	-
2	GOL	C	702	-	-	0/4/4/4	-
2	GOL	A	703	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) 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	C	701	GOL	O1-C1-C2-C3
2	A	701	GOL	O1-C1-C2-O2
2	A	703	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	703	GOL	O2-C2-C3-O3
2	B	701	GOL	O1-C1-C2-O2
2	A	701	GOL	O2-C2-C3-O3
2	A	704	GOL	O1-C1-C2-O2
2	A	704	GOL	O2-C2-C3-O3
2	B	702	GOL	O2-C2-C3-O3
2	C	701	GOL	O1-C1-C2-O2
2	A	704	GOL	C1-C2-C3-O3
2	B	701	GOL	O1-C1-C2-C3

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, 95^{th} 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%)	-0.59	6 (0%) 84 82	18, 30, 66, 102	0
1	B	648/694 (93%)	-0.40	23 (3%) 44 36	18, 31, 85, 119	0
1	C	519/694 (74%)	-0.33	7 (1%) 77 73	20, 32, 57, 83	0
All	All	1823/2082 (87%)	-0.45	36 (1%) 65 60	18, 31, 74, 119	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	TYR	3.5
1	B	588	ALA	3.4
1	B	628	TYR	3.3
1	C	533	TYR	3.2
1	B	10	VAL	3.2
1	B	606	LEU	3.2
1	B	589	PHE	3.1
1	B	629	LEU	3.1
1	A	596	PHE	3.0
1	B	21	PRO	3.0
1	B	614	VAL	2.9
1	B	642	MET	2.8
1	B	592	MET	2.8
1	B	7	ALA	2.7
1	B	11	HIS	2.7
1	B	4	THR	2.7
1	C	484	GLY	2.7
1	B	590	VAL	2.6
1	A	629	LEU	2.6
1	C	48	TYR	2.5
1	C	455	ILE	2.5
1	A	627	ILE	2.4
1	B	14	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	596	PHE	2.4
1	B	8	PRO	2.4
1	A	604	ALA	2.3
1	B	9	GLY	2.3
1	B	591	THR	2.3
1	B	12	HIS	2.2
1	B	575	VAL	2.2
1	B	15	PRO	2.1
1	A	606	LEU	2.1
1	C	488	GLU	2.0
1	C	485	ASN	2.0
1	A	601	THR	2.0
1	C	487	VAL	2.0

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, 95^{th} 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	0.94	0.13	75,79,82,88	0
1	ALY	A	640	12/13	0.97	0.13	27,41,49,55	0

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, 95^{th} 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	B	702	6/6	0.75	0.53	78,85,87,88	0
2	GOL	A	704	6/6	0.79	0.25	67,73,79,84	0
2	GOL	A	702	6/6	0.79	0.60	52,67,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	703	6/6	0.79	0.28	62,74,77,80	0
2	GOL	C	701	6/6	0.80	0.25	69,71,74,78	0
2	GOL	B	701	6/6	0.82	0.37	70,82,84,85	0
2	GOL	C	702	6/6	0.87	0.26	61,63,68,73	0
3	PO4	B	703	5/5	0.93	0.23	80,83,90,94	0
3	PO4	C	703	5/5	0.95	0.20	82,86,88,93	0
3	PO4	A	705	5/5	0.96	0.16	57,61,73,81	0
2	GOL	A	701	6/6	0.96	0.25	46,51,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.