



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:46 PM GMT

PDB ID : 1HM8
Title : CRYSTAL STRUCTURE OF S.PNEUMONIAE N-ACETYLGLUCOSAMIN
E-1-PHOSPHATEURIDYLTRANSFERASE, GLMU, BOUND TO ACETYL
COENZYME A
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Deposited on : 2000-12-05
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

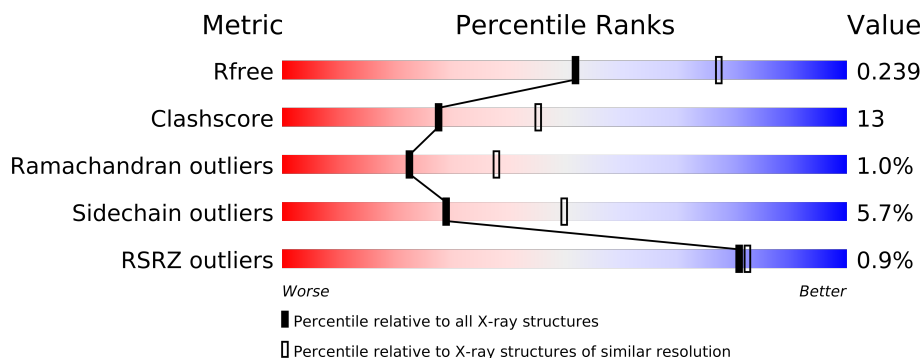
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	468	
1	B	468	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7366 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

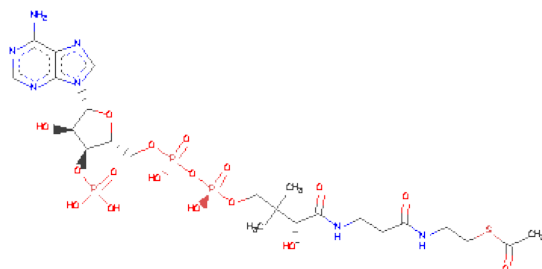
- Molecule 1 is a protein called UDP-N-ACETYLGLUCOSAMINE-1-PHOSPHATEURIDYL-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	6	0
			3495	2188	606	693	8			
1	B	458	Total	C	N	O	S	0	6	0
			3495	2188	606	693	8			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	137	Total	O	0	0
			137	137		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	92.46Å 92.46Å 279.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.63 – 2.50 46.23 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (39.63-2.50) 94.8 (46.23-2.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.84 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.243 0.185 , 0.239	Depositor DCC
R_{free} test set	2926 reflections (10.02%)	DCC
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.5	EDS
Estimated twinning fraction	0.487 for -h-k,k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 29218 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7366	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 8.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: CA, ACO

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	0.56	0/3572	0.76	2/4846 (0.0%)
1	B	0.54	0/3572	0.75	1/4846 (0.0%)
All	All	0.55	0/7144	0.75	3/9692 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	229	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	370	GLU	N-CA-C	-5.40	96.43	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3495	0	3484	89	0
1	B	3495	0	3484	92	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	51	0	34	0	0
3	B	51	0	34	1	0
4	A	133	0	0	5	0
4	B	137	0	0	4	0
All	All	7366	0	7036	181	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (181) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:VAL:HG21	1:A:210:GLU:HB3	1.49	0.93
1:B:124:VAL:HG21	1:B:210:GLU:HB3	1.49	0.92
1:B:72:GLN:HA	1:B:84:MET:HE2	1.54	0.89
1:A:63:LEU:HD23	1:A:63:LEU:H	1.39	0.85
1:B:63:LEU:H	1:B:63:LEU:HD23	1.39	0.85
1:B:37[B]:PHE:HE2	1:B:63:LEU:HD12	1.42	0.84
1:A:72:GLN:HA	1:A:84:MET:HE3	1.60	0.82
1:A:33:LEU:HD23	1:A:63:LEU:HD11	1.59	0.82
1:B:33:LEU:HD23	1:B:63:LEU:HD11	1.63	0.80
1:A:37[B]:PHE:HE2	1:A:63:LEU:HD12	1.51	0.75
1:B:187:ILE:HD13	1:B:200:ASP:HB3	1.71	0.71
1:B:15[A]:ARG:HD2	4:B:2047:HOH:O	1.92	0.69
1:A:144:ASN:HD21	1:A:148:GLU:CD	1.95	0.69
1:A:287:GLY:O	1:A:290:THR:HG23	1.92	0.68
1:B:37[B]:PHE:CE2	1:B:63:LEU:HD12	2.29	0.66
1:B:144:ASN:HD21	1:B:148:GLU:CD	1.98	0.66
1:A:31:SER:OG	1:A:34:GLU:HG3	1.95	0.66
1:B:287:GLY:O	1:B:290:THR:HG23	1.96	0.66
1:B:451:ARG:O	1:B:452:LEU:HD23	1.95	0.64
1:A:187:ILE:HD13	1:A:200:ASP:HB3	1.78	0.64
1:B:31:SER:OG	1:B:34:GLU:HG3	1.97	0.64
1:B:118:HIS:ND1	1:B:126:THR:OG1	2.28	0.64
1:B:179:ARG:HH21	1:B:182:GLU:HB3	1.63	0.63
1:A:419:LEU:C	1:A:419:LEU:HD23	2.19	0.63
1:A:118:HIS:ND1	1:A:126:THR:OG1	2.29	0.62
1:B:419:LEU:C	1:B:419:LEU:HD23	2.20	0.62
1:B:187:ILE:O	1:B:191:ASN:HB2	2.00	0.61
1:A:290:THR:HG21	1:A:304:GLY:O	2.00	0.61
1:A:63:LEU:N	1:A:63:LEU:HD23	2.14	0.61
1:B:385:ASN:O	1:B:391:LYS:HA	2.01	0.61
1:A:451:ARG:O	1:A:452:LEU:HD23	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:37[B]:PHE:CE2	1:A:63:LEU:HD12	2.35	0.60
1:A:332:ARG:HB3	1:A:333:PRO:HD2	1.83	0.60
1:B:146:ASN:HB3	1:B:148:GLU:OE2	2.02	0.60
1:B:168:ILE:C	1:B:168:ILE:HD12	2.22	0.60
1:A:187:ILE:O	1:A:191:ASN:HB2	2.01	0.60
1:A:168:ILE:C	1:A:168:ILE:HD12	2.21	0.60
1:B:61:GLU:HG2	1:B:61:GLU:O	2.00	0.59
1:A:12:LYS:HB2	1:A:75:GLN:OE1	2.01	0.59
1:A:385:ASN:O	1:A:391:LYS:HA	2.02	0.59
1:B:187:ILE:HD13	1:B:200:ASP:CB	2.33	0.59
1:A:146:ASN:HB3	1:A:148:GLU:OE2	2.03	0.59
1:A:179:ARG:HH21	1:A:182:GLU:HB3	1.66	0.58
1:A:123:ASN:HD21	1:A:211:LYS:NZ	2.02	0.58
1:A:61:GLU:HG2	1:A:61:GLU:O	2.02	0.58
1:A:332:ARG:HB3	1:A:333:PRO:CD	2.33	0.58
1:B:332:ARG:HB3	1:B:333:PRO:HD2	1.86	0.58
1:B:53:GLY:O	1:B:56:ALA:HB2	2.03	0.58
1:A:53:GLY:O	1:A:56:ALA:HB2	2.04	0.58
1:B:332:ARG:HB3	1:B:333:PRO:CD	2.34	0.58
1:B:12:LYS:HB2	1:B:75:GLN:OE1	2.04	0.58
1:A:15[A]:ARG:HD2	4:A:1111:HOH:O	2.03	0.57
1:A:270:PRO:HD2	4:A:1031:HOH:O	2.05	0.57
1:A:6:ILE:HD13	1:A:82:VAL:HG13	1.85	0.57
1:A:229:ARG:HA	1:A:232:LEU:HB2	1.86	0.57
1:B:63:LEU:HD23	1:B:63:LEU:N	2.13	0.56
1:B:290:THR:HG21	1:B:304:GLY:O	2.05	0.56
1:A:63:LEU:C	1:A:65:GLY:H	2.09	0.55
1:A:441:ARG:HD2	4:A:1118:HOH:O	2.06	0.55
1:B:63:LEU:C	1:B:65:GLY:H	2.09	0.55
1:B:334:ASN:O	1:B:351:GLY:HA2	2.06	0.55
1:B:123:ASN:HD22	1:B:211:LYS:HD3	1.72	0.55
1:A:143:ARG:HA	1:A:148:GLU:O	2.07	0.54
1:A:16:MET:HG3	1:A:22:LYS:HG3	1.88	0.54
1:B:229:ARG:HA	1:B:232:LEU:HB2	1.88	0.54
1:A:385:ASN:HD22	1:A:385:ASN:H	1.56	0.54
1:B:16:MET:HG3	1:B:22:LYS:HG3	1.89	0.54
1:A:168:ILE:HD12	1:A:168:ILE:O	2.08	0.54
1:A:187:ILE:HD13	1:A:200:ASP:CB	2.37	0.54
1:A:334:ASN:O	1:A:351:GLY:HA2	2.07	0.53
1:A:39[A]:SER:HB3	1:A:111:LEU:HD22	1.89	0.53
1:B:6:ILE:HD13	1:B:82:VAL:HG13	1.90	0.53
1:B:72:GLN:HA	1:B:84:MET:CE	2.33	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:143:ARG:HA	1:B:148:GLU:O	2.08	0.53
1:A:116:ASP:O	1:A:120:ASN:HB2	2.07	0.53
1:A:362:HIS:N	1:A:362:HIS:CD2	2.77	0.53
1:B:43:ILE:HD12	1:B:115:ILE:HD11	1.90	0.53
1:A:141:ILE:HG13	1:A:167:GLU:HG2	1.91	0.52
1:A:123:ASN:HD22	1:A:211:LYS:HD3	1.75	0.51
1:B:43:ILE:HB	1:B:115:ILE:HD12	1.93	0.51
1:B:128:LEU:HD11	1:B:217:LEU:HG	1.92	0.51
1:A:164:GLN:O	1:A:166:LYS:HD2	2.10	0.51
1:B:385:ASN:HD22	1:B:385:ASN:H	1.58	0.51
1:B:168:ILE:HD12	1:B:168:ILE:O	2.10	0.51
1:B:123:ASN:HD21	1:B:211:LYS:NZ	2.08	0.51
1:A:62:VAL:HB	1:A:63:LEU:HD23	1.93	0.51
1:A:287:GLY:O	1:A:290:THR:CG2	2.59	0.51
1:B:62:VAL:HB	1:B:63:LEU:HD23	1.92	0.51
1:A:126:THR:HA	1:A:213:GLY:O	2.11	0.51
1:A:43:ILE:HD12	1:A:115:ILE:HD11	1.93	0.51
1:B:116:ASP:O	1:B:120:ASN:HB2	2.10	0.51
1:A:86:GLU:HB3	1:A:87:PRO:HD3	1.93	0.51
1:A:128:LEU:HD11	1:A:217:LEU:HG	1.93	0.50
1:B:362:HIS:CD2	1:B:362:HIS:N	2.78	0.50
1:B:261:TYR:CD1	1:B:261:TYR:N	2.78	0.50
1:B:287:GLY:O	1:B:290:THR:CG2	2.59	0.50
1:B:164:GLN:O	1:B:166:LYS:HD2	2.11	0.50
1:A:362:HIS:CD2	1:A:379:ALA:HB2	2.47	0.49
1:B:144:ASN:ND2	1:B:148:GLU:HB2	2.28	0.49
1:B:362:HIS:CD2	1:B:379:ALA:HB2	2.48	0.49
1:B:80:HIS:O	1:B:84:MET:HG2	2.13	0.48
1:A:179:ARG:NH2	1:A:182:GLU:HB3	2.29	0.48
1:A:361:GLY:C	1:A:362:HIS:CG	2.86	0.48
1:B:141:ILE:HG13	1:B:167:GLU:HG2	1.95	0.48
1:B:361:GLY:C	1:B:362:HIS:CG	2.87	0.48
1:B:52:VAL:HG22	1:B:53:GLY:N	2.29	0.48
1:A:80:HIS:O	1:A:84:MET:HG2	2.14	0.48
1:A:123:ASN:HD21	1:A:211:LYS:HZ2	1.60	0.48
1:B:33:LEU:CD2	1:B:63:LEU:HD11	2.41	0.47
1:B:179:ARG:NH2	1:B:182:GLU:HB3	2.28	0.47
1:A:63:LEU:CD2	1:A:63:LEU:H	2.17	0.47
1:B:144:ASN:O	1:B:147:ALA:N	2.42	0.47
1:B:126:THR:HA	1:B:213:GLY:O	2.14	0.47
1:A:43:ILE:HB	1:A:115:ILE:HD12	1.95	0.47
1:A:144:ASN:O	1:A:147:ALA:N	2.42	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:GLU:HB3	1:B:87:PRO:HD3	1.96	0.47
1:A:144:ASN:ND2	1:A:148:GLU:HB2	2.30	0.47
1:B:227:ASN:HB2	4:B:2127:HOH:O	2.14	0.47
1:B:347:VAL:HG22	1:B:364:THR:HB	1.97	0.46
1:A:72:GLN:HA	1:A:84:MET:CE	2.38	0.46
1:B:63:LEU:H	1:B:63:LEU:CD2	2.17	0.46
1:B:121:HIS:N	1:B:121:HIS:ND1	2.64	0.46
1:A:54:HIS:C	1:A:56:ALA:N	2.69	0.46
1:B:375:VAL:HG12	1:B:376:ASN:N	2.30	0.46
1:A:33:LEU:CD2	1:A:63:LEU:HD11	2.40	0.46
1:A:86:GLU:HG2	1:A:90:GLU:HB2	1.98	0.46
1:A:128:LEU:HB3	1:A:172:THR:HB	1.99	0.45
1:A:196:TYR:N	1:A:196:TYR:CD1	2.84	0.45
1:B:128:LEU:HB3	1:B:172:THR:HB	1.99	0.45
1:B:208:THR:OG1	1:B:210:GLU:HG3	2.17	0.45
1:A:419:LEU:HD23	1:A:420:VAL:N	2.32	0.45
1:A:52:VAL:HG22	1:A:53:GLY:N	2.32	0.45
1:A:141:ILE:CG1	1:A:167:GLU:HG2	2.46	0.45
1:A:121:HIS:N	1:A:121:HIS:ND1	2.65	0.45
1:A:375:VAL:HG12	1:A:376:ASN:N	2.32	0.45
1:B:270:PRO:O	1:B:271:GLU:HB2	2.17	0.45
1:B:191:ASN:HB3	4:B:2085:HOH:O	2.17	0.44
1:B:419:LEU:HD23	1:B:420:VAL:N	2.33	0.44
1:B:78:THR:O	1:B:82:VAL:HG23	2.17	0.44
1:B:183:ALA:O	1:B:187:ILE:HG13	2.17	0.44
1:A:376:ASN:ND2	4:A:1084:HOH:O	2.42	0.44
1:B:196:TYR:N	1:B:196:TYR:CD1	2.86	0.44
1:B:127:ILE:O	1:B:214:ALA:HA	2.18	0.44
1:A:261:TYR:CD1	1:A:261:TYR:N	2.83	0.44
1:A:385:ASN:ND2	1:A:385:ASN:H	2.16	0.44
1:A:55:LYS:HA	1:A:57:GLU:OE2	2.18	0.44
1:B:54:HIS:C	1:B:56:ALA:N	2.70	0.43
1:A:127:ILE:O	1:A:214:ALA:HA	2.18	0.43
1:A:270:PRO:O	1:A:271:GLU:HB2	2.18	0.43
1:A:264:ILE:HG23	1:A:265:ASP:N	2.33	0.43
1:A:455:HIS:HA	1:A:456:PRO:HD3	1.90	0.43
1:B:144:ASN:HD21	1:B:148:GLU:HB2	1.84	0.43
1:B:141:ILE:CG1	1:B:167:GLU:HG2	2.48	0.43
1:B:381:THR:HG22	1:B:382:ILE:N	2.33	0.43
1:B:55:LYS:HA	1:B:57:GLU:OE2	2.18	0.43
1:B:385:ASN:ND2	1:B:385:ASN:H	2.17	0.43
1:A:144:ASN:O	1:A:146:ASN:N	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:58:LEU:O	1:A:62:VAL:HG23	2.19	0.43
1:B:376:ASN:ND2	4:B:2093:HOH:O	2.48	0.43
1:B:39[A]:SER:HB3	1:B:111:LEU:HD22	2.01	0.43
1:A:208:THR:OG1	1:A:210:GLU:HG3	2.18	0.42
1:B:124:VAL:HA	1:B:176:ASP:OD2	2.19	0.42
1:A:362:HIS:O	1:A:363:LEU:C	2.58	0.42
1:B:350:LYS:O	1:B:367:GLY:HA2	2.20	0.42
1:B:144:ASN:O	1:B:146:ASN:N	2.53	0.42
1:A:191:ASN:HB3	4:A:1083:HOH:O	2.20	0.42
1:A:111:LEU:HA	1:A:111:LEU:HD12	1.87	0.42
1:B:20:LEU:HD12	1:B:21:PRO:HD2	2.02	0.42
1:A:381:THR:HG22	1:A:382:ILE:N	2.34	0.41
1:B:86:GLU:HG2	1:B:90:GLU:HB2	2.02	0.41
1:A:124:VAL:HA	1:A:176:ASP:OD2	2.21	0.41
1:B:76:LEU:HB2	1:B:80:HIS:ND1	2.36	0.41
1:B:58:LEU:O	1:B:62:VAL:HG23	2.21	0.41
1:B:65:GLY:O	1:B:67:THR:HG22	2.21	0.41
1:B:385:ASN:HD22	1:B:385:ASN:N	2.16	0.41
1:A:290:THR:HB	1:A:307:ALA:H	1.85	0.41
1:A:144:ASN:HD21	1:A:148:GLU:HB2	1.86	0.40
1:B:264:ILE:HG23	1:B:265:ASP:N	2.36	0.40
1:B:384:VAL:HA	3:B:2900:ACO:HH32	2.03	0.40
1:B:362:HIS:O	1:B:363:LEU:C	2.59	0.40
1:A:20:LEU:HD12	1:A:21:PRO:HD2	2.04	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	462/468 (99%)	430 (93%)	27 (6%)	5 (1%)	21	34
1	B	462/468 (99%)	426 (92%)	32 (7%)	4 (1%)	25	42
All	All	924/936 (99%)	856 (93%)	59 (6%)	9 (1%)	22	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLY
1	A	66	GLN
1	A	145	ASP
1	B	11	GLY
1	B	66	GLN
1	B	145	ASP
1	A	333	PRO
1	B	333	PRO
1	A	65	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	383/386 (99%)	362 (94%)	21 (6%)	30	52
1	B	383/386 (99%)	361 (94%)	22 (6%)	29	50
All	All	766/772 (99%)	723 (94%)	43 (6%)	29	51

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	63	LEU
1	A	66	GLN
1	A	111	LEU
1	A	120	ASN
1	A	121	HIS
1	A	150	LEU
1	A	173	TYR
1	A	179	ARG
1	A	196	TYR
1	A	232	LEU
1	A	246	LYS
1	A	283	GLN
1	A	290	THR
1	A	294	ASN

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Mol	Chain	Res	Type
1	A	311	ASN
1	A	345	ASN
1	A	359	LYS
1	A	362	HIS
1	A	376	ASN
1	A	385	ASN
1	B	8	LEU
1	B	17	LYS
1	B	63	LEU
1	B	66	GLN
1	B	111	LEU
1	B	120	ASN
1	B	121	HIS
1	B	150	LEU
1	B	173	TYR
1	B	179	ARG
1	B	196	TYR
1	B	232	LEU
1	B	246	LYS
1	B	283	GLN
1	B	290	THR
1	B	294	ASN
1	B	311	ASN
1	B	345	ASN
1	B	359	LYS
1	B	362	HIS
1	B	376	ASN
1	B	385	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	120	ASN
1	A	123	ASN
1	A	193	GLN
1	A	277	ASN
1	A	294	ASN
1	A	311	ASN
1	A	345	ASN
1	A	385	ASN
1	B	113	ASN

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Mol	Chain	Res	Type
1	B	120	ASN
1	B	123	ASN
1	B	193	GLN
1	B	250	ASN
1	B	277	ASN
1	B	294	ASN
1	B	311	ASN
1	B	345	ASN
1	B	385	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
3	ACO	A	1900	-	53,53,53	1.53	7 (13%)	79,79,79	1.28	9 (11%)
3	ACO	B	2900	-	53,53,53	1.56	7 (13%)	79,79,79	1.29	10 (12%)

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
3	ACO	A	1900	-	-	0/51/67/67	0/1/3/3
3	ACO	B	2900	-	-	0/51/67/67	0/1/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1900	ACO	C-S1P	-5.76	1.50	1.75
3	B	2900	ACO	C-S1P	-5.72	1.50	1.75
3	B	2900	ACO	CBP-CAP	4.25	1.60	1.55
3	A	1900	ACO	C8A-N9A	3.35	1.41	1.36
3	A	1900	ACO	CBP-CAP	3.35	1.59	1.55
3	B	2900	ACO	C8A-N9A	3.04	1.41	1.36
3	B	2900	ACO	CCP-CBP	-3.04	1.47	1.52
3	B	2900	ACO	C4A-N3A	3.00	1.40	1.35
3	A	1900	ACO	C4A-N3A	2.97	1.40	1.35
3	A	1900	ACO	CCP-CBP	-2.38	1.49	1.52
3	A	1900	ACO	CH3-C	2.27	1.59	1.50
3	B	2900	ACO	OAP-CAP	2.17	1.46	1.42
3	A	1900	ACO	C8A-N7A	-2.07	1.30	1.34
3	B	2900	ACO	CH3-C	2.06	1.58	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2900	ACO	C2P-S1P-C	4.11	118.07	101.38
3	A	1900	ACO	C2P-S1P-C	4.06	117.87	101.38
3	A	1900	ACO	CCP-CBP-CAP	-3.55	103.51	108.70
3	A	1900	ACO	CEP-CBP-CAP	3.45	114.80	108.82
3	B	2900	ACO	CDP-CBP-CCP	3.39	113.64	108.76
3	A	1900	ACO	CDP-CBP-CCP	3.35	113.58	108.76
3	B	2900	ACO	CCP-CBP-CAP	-3.32	103.84	108.70
3	B	2900	ACO	CEP-CBP-CAP	3.24	114.43	108.82
3	A	1900	ACO	C4B-O4B-C1B	3.13	113.15	109.75
3	B	2900	ACO	C4B-O4B-C1B	3.08	113.09	109.75
3	A	1900	ACO	N3A-C2A-N1A	-2.70	126.45	128.71
3	B	2900	ACO	C4A-C5A-N7A	2.42	111.60	109.52
3	A	1900	ACO	C4A-C5A-N7A	2.31	111.50	109.52
3	B	2900	ACO	N3A-C2A-N1A	-2.30	126.78	128.71
3	A	1900	ACO	C2P-C3P-N4P	-2.27	107.36	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2900	ACO	C2P-C3P-N4P	-2.26	107.40	112.50
3	A	1900	ACO	C2B-C3B-C4B	2.10	107.25	103.16
3	B	2900	ACO	C2B-C3B-C4B	2.08	107.22	103.16
3	B	2900	ACO	C8A-N9A-C4A	-2.06	105.33	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	458/468 (97%)	-0.32	3 (0%) 84 86	15, 32, 68, 79	0
1	B	458/468 (97%)	-0.35	5 (1%) 77 79	15, 32, 68, 79	0
All	All	916/936 (97%)	-0.34	8 (0%) 81 82	15, 32, 68, 79	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	HIS	4.1
1	B	66	GLN	3.2
1	B	12	LYS	2.7
1	A	54	HIS	2.3
1	A	66	GLN	2.2
1	B	61	GLU	2.2
1	A	146	ASN	2.1
1	B	145	ASP	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ACO	B	2900	51/51	0.13	0.45	36,44,50,51	0
3	ACO	A	1900	51/51	0.12	0.18	36,45,50,52	0
2	CA	B	2902	1/1	0.11	-0.45	54,54,54,54	1
2	CA	B	2901	1/1	0.09	-0.89	64,64,64,64	0
2	CA	A	1901	1/1	0.02	-20.85	58,58,58,58	0
2	CA	A	1902	1/1	0.03	-201.00	51,51,51,51	1

6.5 Other polymers ⓘ

There are no such residues in this entry.