



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 11:46 PM GMT

PDB ID : 1Z8D  
Title : Crystal Structure of Human Muscle Glycogen Phosphorylase a with AMP and Glucose  
Authors : Lukacs, C.M.; Oikonomakos, N.G.; Crowther, R.L.; Hong, L.N.; Kammlott, R.U.; Levin, W.; Li, S.; Liu, C.M.; Lucas-McGady, D.; Pietranico, S.; Reik, L.  
Deposited on : 2005-03-30  
Resolution : 2.30 Å(reported)

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

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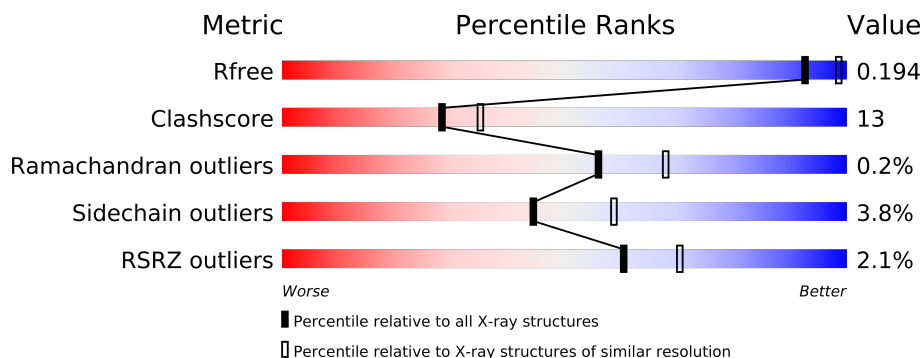
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 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	842	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	ADE	A	902	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7121 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.

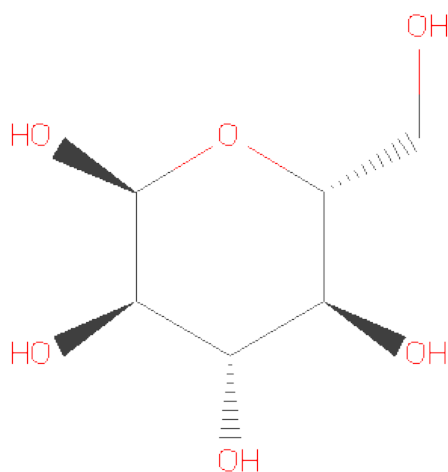
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	821	6707	4267	1187	1221	2	30	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SEP	SER	ENGINEERED	UNP P11217
A	680	LLP	LYS	ENGINEERED	UNP P11217

- Molecule 2 is AMP (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



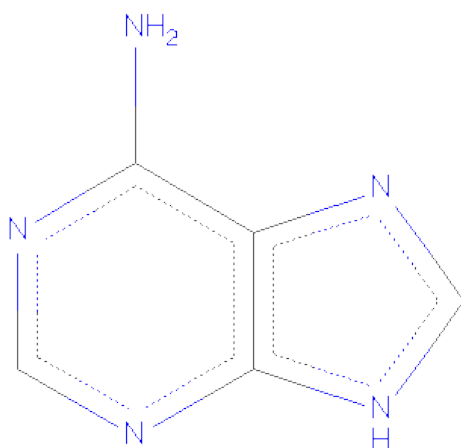
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is ADENINE (three-letter code: ADE) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			10	5	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	369	Total 369	O 369	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.37Å 144.00Å 59.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.79 – 2.30 30.79 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.79-2.30) 97.7 (30.79-2.27)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.26Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, $R_{free}$	0.192 , 0.251 0.194 , 0.194	Depositor DCC
$R_{free}$ test set	934 reflections (2.63%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 21.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36505 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, AMP, ADE, LLP, SEP

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	0.34	0/6822	0.60	1/9224 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	558	ASN	N-CA-C	-5.81	95.31	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	SEP	CA

There are no planarity outliers.

### 5.2 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 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	6707	0	6636	169	1
2	A	12	0	12	0	0
3	A	23	0	12	0	0
4	A	10	0	4	0	0
5	A	369	0	0	7	0
All	All	7121	0	6664	169	1

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:549:LEU:HG	1:A:555:VAL:HG21	1.46	0.97
1:A:549:LEU:HB3	1:A:555:VAL:HG11	1.50	0.92
1:A:455:VAL:H	1:A:459:HIS:HD2	1.25	0.82
1:A:21:VAL:HG13	1:A:23:ASN:HB2	1.61	0.82
1:A:549:LEU:CG	1:A:555:VAL:HG21	2.12	0.80
1:A:546:ALA:HB1	1:A:557:ILE:HG13	1.63	0.80
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.65	0.77
1:A:235:ASN:HA	1:A:833:ARG:CG	2.16	0.75
1:A:455:VAL:HG22	1:A:484:ASN:OD1	1.85	0.74
1:A:558:ASN:O	1:A:560:ASN:N	2.20	0.72
1:A:554:LYS:HD3	1:A:555:VAL:N	2.04	0.72
1:A:311:PHE:CZ	1:A:323:ARG:HD3	2.25	0.72
1:A:591:LYS:HE2	1:A:633:ASP:OD2	1.90	0.71
1:A:565:ILE:HD12	1:A:660:ALA:HB2	1.72	0.71
1:A:287:GLU:HG2	1:A:289:LYS:HG2	1.74	0.70
1:A:565:ILE:HD13	1:A:656:VAL:HG22	1.74	0.70
1:A:355:ASP:OD2	1:A:398:ARG:HD3	1.93	0.69
1:A:100:VAL:HG21	1:A:494:LEU:HD21	1.75	0.68
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.76	0.67
1:A:16:ARG:NE	1:A:16:ARG:HA	2.11	0.65
1:A:7:GLN:HG3	1:A:8:GLU:N	2.11	0.65
1:A:455:VAL:HG13	1:A:674:SER:HB2	1.80	0.64
1:A:96:GLN:HG2	1:A:494:LEU:HD22	1.78	0.64
1:A:546:ALA:CB	1:A:557:ILE:HG21	2.27	0.64
1:A:22:GLU:OE1	1:A:104:LEU:HD21	1.98	0.64
1:A:550:GLU:HB2	1:A:555:VAL:HG12	1.79	0.64
1:A:687:LEU:HD13	1:A:800:MET:HE1	1.79	0.63
1:A:33:ARG:HG3	1:A:37:PHE:HD2	1.64	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:VAL:HG13	1:A:674:SER:CB	2.30	0.62
1:A:235:ASN:ND2	1:A:237:VAL:H	1.97	0.62
1:A:647:ASN:ND2	1:A:649:ARG:HE	1.97	0.62
1:A:12:GLN:O	1:A:14:SEP:N	2.33	0.61
1:A:455:VAL:HG22	1:A:484:ASN:CG	2.20	0.61
1:A:554:LYS:HD3	1:A:555:VAL:H	1.65	0.61
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.83	0.61
1:A:557:ILE:HD13	1:A:557:ILE:N	2.16	0.61
1:A:386:ARG:HD2	1:A:432:GLU:OE1	2.01	0.60
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.84	0.60
1:A:558:ASN:C	1:A:560:ASN:H	2.04	0.60
1:A:68:ILE:O	1:A:72:GLN:HG3	2.01	0.59
1:A:5:SER:OG	1:A:7:GLN:HG2	2.03	0.59
1:A:565:ILE:HD13	1:A:656:VAL:CG2	2.33	0.58
1:A:82:ILE:HD13	1:A:825:TRP:CE3	2.39	0.58
1:A:636:VAL:O	1:A:639:ARG:HD3	2.06	0.56
1:A:413:ARG:HD3	5:A:1258:HOH:O	2.05	0.56
1:A:192:ALA:HB1	1:A:224:MET:CE	2.36	0.56
1:A:246:ALA:O	1:A:247:LYS:HD3	2.07	0.55
1:A:741:VAL:HA	1:A:744:GLN:HE21	1.70	0.55
1:A:490:ARG:HA	1:A:494:LEU:HG	1.87	0.55
1:A:532:ARG:HG2	1:A:532:ARG:HH11	1.72	0.55
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.88	0.55
1:A:546:ALA:HB1	1:A:557:ILE:HG21	1.88	0.55
1:A:557:ILE:HD13	1:A:557:ILE:H	1.72	0.55
1:A:517:GLN:NE2	1:A:520:LYS:HE3	2.22	0.55
1:A:545:PHE:O	1:A:549:LEU:HB2	2.07	0.54
1:A:311:PHE:CE1	1:A:323:ARG:HD3	2.42	0.54
1:A:454:GLY:HA3	1:A:460:SER:OG	2.07	0.54
1:A:575:ARG:HD3	1:A:666:ILE:O	2.06	0.54
1:A:274:ASN:HA	1:A:277:ARG:CG	2.38	0.54
1:A:469:LYS:O	1:A:473:GLU:HG3	2.08	0.54
1:A:311:PHE:O	1:A:323:ARG:HD2	2.08	0.53
1:A:542:LYS:CE	1:A:661:ASP:OD2	2.57	0.53
1:A:555:VAL:HG13	1:A:556:HIS:N	2.23	0.53
1:A:35:LEU:HD13	1:A:35:LEU:O	2.09	0.53
1:A:547:ALA:O	1:A:551:ARG:HG2	2.08	0.53
1:A:6:ASP:O	1:A:10:ARG:HG3	2.09	0.53
1:A:35:LEU:HD13	1:A:35:LEU:C	2.29	0.52
1:A:617:LYS:HD3	5:A:1270:HOH:O	2.08	0.52
1:A:405:GLU:O	1:A:409:ARG:HG2	2.08	0.52
1:A:388:PRO:HB2	1:A:390:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:VAL:O	1:A:16:ARG:HG2	2.09	0.52
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.91	0.52
1:A:538:LYS:CE	1:A:660:ALA:O	2.58	0.52
1:A:682:MET:HE1	1:A:699:MET:HG2	1.91	0.52
1:A:517:GLN:HE21	1:A:520:LYS:HE3	1.76	0.51
1:A:517:GLN:HG2	5:A:1162:HOH:O	2.09	0.51
1:A:546:ALA:HB1	1:A:557:ILE:CG1	2.36	0.51
1:A:830:SER:OG	1:A:832:GLN:HG2	2.11	0.51
1:A:598:PHE:HD2	1:A:639:ARG:HH21	1.59	0.51
1:A:16:ARG:HA	1:A:16:ARG:HE	1.74	0.50
1:A:458:ILE:O	1:A:462:ILE:HG13	2.11	0.50
1:A:622:LEU:HD22	1:A:626:ILE:HG13	1.94	0.50
1:A:192:ALA:HB1	1:A:224:MET:HE2	1.92	0.49
1:A:23:ASN:HB3	1:A:26:GLU:H	1.78	0.49
1:A:538:LYS:HE2	1:A:660:ALA:O	2.11	0.49
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.34	0.49
1:A:81:ARG:NE	1:A:310:ARG:HD3	2.28	0.49
1:A:177:GLU:CD	1:A:177:GLU:H	2.15	0.49
1:A:274:ASN:HA	1:A:277:ARG:HG3	1.96	0.48
1:A:21:VAL:HG12	1:A:26:GLU:HG3	1.96	0.48
1:A:532:ARG:NH1	1:A:533:ASP:OD1	2.47	0.48
1:A:833:ARG:HD3	1:A:833:ARG:N	2.29	0.48
1:A:303:THR:O	1:A:307:ILE:HG13	2.13	0.48
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.95	0.47
1:A:67:TRP:HA	1:A:238:VAL:HB	1.97	0.47
1:A:21:VAL:CG1	1:A:26:GLU:HG3	2.45	0.47
1:A:713:MET:HG3	1:A:776:ASP:OD1	2.15	0.47
1:A:119:MET:O	1:A:123:GLU:HG3	2.14	0.47
1:A:21:VAL:CG1	1:A:23:ASN:HB2	2.41	0.47
1:A:291:LEU:O	1:A:295:GLN:HG3	2.14	0.46
1:A:143:PHE:O	1:A:147:MET:HG3	2.16	0.46
1:A:4:LEU:O	1:A:9:LYS:HE3	2.15	0.46
1:A:67:TRP:HD1	1:A:238:VAL:HG12	1.80	0.46
1:A:525:VAL:O	1:A:799:ARG:HD2	2.16	0.46
1:A:378:THR:HG22	5:A:1095:HOH:O	2.16	0.46
1:A:62:HIS:O	1:A:66:ARG:HG2	2.16	0.46
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.97	0.46
1:A:194:PRO:HB3	1:A:224:MET:HE1	1.98	0.45
1:A:60:ARG:HD2	1:A:188:PRO:O	2.16	0.45
1:A:311:PHE:CE2	1:A:323:ARG:HD3	2.51	0.45
1:A:4:LEU:HG	1:A:8:GLU:HG2	1.97	0.45
1:A:514:ASP:O	1:A:517:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21:VAL:C	1:A:23:ASN:H	2.19	0.45
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.99	0.45
1:A:60:ARG:O	1:A:64:VAL:HG23	2.16	0.45
1:A:235:ASN:CA	1:A:833:ARG:HG3	2.41	0.44
1:A:587:TYR:CD1	1:A:630:VAL:HG22	2.52	0.44
1:A:66:ARG:HB2	1:A:238:VAL:HG21	1.99	0.44
1:A:411:LEU:HA	1:A:411:LEU:HD12	1.78	0.44
1:A:457:ARG:HH22	1:A:701:GLU:CD	2.21	0.44
1:A:692:MET:HG3	1:A:714:ARG:NE	2.33	0.44
1:A:227:ASP:OD1	1:A:242:ARG:CD	2.66	0.44
1:A:740:GLN:O	1:A:744:GLN:HG3	2.18	0.44
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.18	0.43
1:A:558:ASN:C	1:A:560:ASN:N	2.69	0.43
1:A:575:ARG:NH2	1:A:776:ASP:OD2	2.36	0.43
1:A:557:ILE:CD1	1:A:557:ILE:N	2.81	0.43
1:A:45:VAL:O	1:A:45:VAL:HG22	2.18	0.43
1:A:515:LEU:HD22	1:A:812:SER:HB2	2.00	0.43
1:A:94:THR:HG23	5:A:963:HOH:O	2.19	0.43
1:A:351:ARG:CD	1:A:398:ARG:HG2	2.49	0.43
1:A:397:PRO:O	1:A:401:GLN:HG3	2.19	0.43
1:A:455:VAL:HG13	1:A:674:SER:HB3	2.00	0.43
1:A:235:ASN:HD22	1:A:236:ASN:N	2.17	0.43
1:A:555:VAL:CG1	1:A:556:HIS:N	2.81	0.42
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.02	0.42
1:A:235:ASN:H	1:A:235:ASN:HD22	1.66	0.42
1:A:538:LYS:HD2	1:A:538:LYS:HA	1.79	0.42
1:A:183:LEU:HB2	5:A:971:HOH:O	2.19	0.42
1:A:815:ARG:HD2	1:A:815:ARG:C	2.40	0.42
1:A:605:ILE:O	1:A:644:PHE:HA	2.20	0.42
1:A:546:ALA:CB	1:A:557:ILE:HG13	2.41	0.42
1:A:361:TRP:CH2	1:A:405:GLU:HG2	2.55	0.42
1:A:522:LEU:HD13	1:A:806:ALA:CB	2.50	0.42
1:A:589:ARG:HD2	1:A:737:GLU:OE2	2.19	0.42
1:A:103:ALA:HB2	1:A:234:ARG:HD2	2.02	0.41
1:A:336:GLN:OE1	1:A:373:ALA:HB3	2.20	0.41
1:A:138:ARG:HD2	1:A:138:ARG:HA	1.88	0.41
1:A:517:GLN:NE2	1:A:520:LYS:CE	2.83	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.92	0.41
1:A:21:VAL:O	1:A:23:ASN:N	2.43	0.41
1:A:235:ASN:HA	1:A:833:ARG:HG2	1.99	0.41
1:A:386:ARG:NH1	1:A:432:GLU:OE2	2.53	0.41
1:A:548:TYR:CD1	1:A:548:TYR:C	2.93	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:633:ASP:HA	1:A:634:PRO:HD2	1.96	0.41
1:A:33:ARG:HG3	1:A:37:PHE:CD2	2.50	0.41
1:A:390:HIS:HA	5:A:927:HOH:O	2.20	0.41
1:A:421:ASP:OD1	1:A:424:ARG:HB2	2.21	0.41
1:A:13:ILE:O	1:A:14:SEP:CB	2.69	0.41
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.51	0.41
1:A:455:VAL:HG22	1:A:484:ASN:ND2	2.35	0.41
1:A:157:TYR:CE2	1:A:242:ARG:HG2	2.56	0.41
1:A:682:MET:HE1	1:A:811:PHE:CD2	2.56	0.41
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.50	0.41
1:A:706:GLU:CD	1:A:706:GLU:H	2.23	0.41
1:A:351:ARG:HD2	1:A:398:ARG:HG2	2.02	0.40
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.03	0.40
1:A:568:LYS:HB3	1:A:568:LYS:HE2	1.90	0.40
1:A:455:VAL:CG2	1:A:484:ASN:OD1	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:270:ASN:ND2	1:A:270:ASN:ND2[2_655]	1.71	0.49

## 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	813/842 (97%)	777 (96%)	34 (4%)	2 (0%)	56 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	559	PRO
1	A	13	ILE

### 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	710/727 (98%)	683 (96%)	27 (4%)	44 59

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	63	LEU
1	A	90	TYR
1	A	95	LEU
1	A	128	ASP
1	A	211	GLN
1	A	235	ASN
1	A	242	ARG
1	A	277	ARG
1	A	291	LEU
1	A	337	LEU
1	A	384	LEU
1	A	400	LEU
1	A	411	LEU
1	A	425	LEU
1	A	455	VAL
1	A	492	LEU
1	A	522	LEU
1	A	557	ILE
1	A	579	ASN
1	A	613	TYR
1	A	622	LEU
1	A	649	ARG
1	A	683	LEU
1	A	706	GLU
1	A	708	PHE
1	A	831	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	97	ASN
1	A	211	GLN
1	A	235	ASN
1	A	239	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	517	GLN
1	A	558	ASN
1	A	566	GLN
1	A	579	ASN
1	A	588	ASN
1	A	744	GLN
1	A	763	ASN
1	A	832	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	SEP	A	14	1	9,9,10	5.93	4 (44%)	10,12,14	1.09	1 (10%)
1	LLP	A	680	1	24,24,25	3.96	7 (29%)	30,32,34	3.12	12 (40%)

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	SEP	A	14	1	1/1/2/3	0/6/8/10	0/0/0/0
1	LLP	A	680	1	-	0/15/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O-C	17.93	1.23	1.11
1	A	14	SEP	O-C	16.95	1.23	1.11
1	A	14	SEP	P-OG	-3.59	1.47	1.60
1	A	680	LLP	C4'-C4	2.93	1.55	1.51
1	A	680	LLP	C3-C2	-2.86	1.38	1.40
1	A	680	LLP	C2-N1	2.84	1.39	1.33
1	A	14	SEP	CA-C	2.60	1.53	1.48
1	A	680	LLP	CA-C	2.40	1.52	1.48
1	A	14	SEP	P-O3P	-2.25	1.46	1.54
1	A	680	LLP	C5-C4	2.15	1.43	1.40
1	A	680	LLP	P-OP3	-2.07	1.47	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	OP3-P-OP1	-7.94	84.50	110.44
1	A	680	LLP	OP3-P-OP4	-7.92	84.78	106.65
1	A	680	LLP	OP3-P-OP2	-5.38	86.66	107.61
1	A	680	LLP	C4-C4'-NZ	4.54	119.97	111.52
1	A	680	LLP	OP2-P-OP4	4.14	118.08	106.65
1	A	680	LLP	C2'-C2-C3	4.11	126.01	121.02
1	A	680	LLP	C-CA-N	-4.06	109.77	113.83
1	A	680	LLP	OP2-P-OP1	3.72	122.59	110.44
1	A	680	LLP	OP4-P-OP1	3.63	117.35	106.71
1	A	680	LLP	OP4-C5'-C5	3.31	115.98	109.26
1	A	680	LLP	C6-C5-C4	-2.69	116.06	118.10
1	A	14	SEP	O3P-P-O2P	2.32	116.64	107.61
1	A	680	LLP	C4-C3-C2	2.02	123.31	119.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	SEP	CA

There are no torsion outliers.

There are no ring outliers.



## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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	AMP	A	900	-	25,25,25	2.21	7 (28%)	38,38,38	1.69	6 (15%)
2	GLC	A	901	-	12,12,12	0.35	0	17,17,17	0.34	0
4	ADE	A	902	-	11,11,11	1.96	3 (27%)	15,15,15	3.02	8 (53%)

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	AMP	A	900	-	-	0/10/26/26	0/1/3/3
2	GLC	A	901	-	-	0/2/22/22	0/1/1/1
4	ADE	A	902	-	-	0/0/0/0	0/0/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	AMP	C2'-C1'	6.50	1.62	1.53
3	A	900	AMP	C3'-C4'	5.27	1.67	1.53
4	A	902	ADE	C8-N9	5.18	1.42	1.34
3	A	900	AMP	C8-N9	3.37	1.41	1.36
3	A	900	AMP	O3'-C3'	3.34	1.51	1.43
3	A	900	AMP	C2'-C3'	2.71	1.60	1.53
3	A	900	AMP	O4'-C1'	2.25	1.44	1.41
4	A	902	ADE	C8-N7	2.17	1.39	1.34
4	A	902	ADE	C2-N3	2.08	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	AMP	C2-N3	2.08	1.36	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	ADE	C5-C4-N9	5.75	111.68	106.07
4	A	902	ADE	C8-N9-C4	-5.71	100.56	107.69
3	A	900	AMP	C4-C5-N7	4.97	113.78	109.52
4	A	902	ADE	N3-C2-N1	-4.62	124.84	128.71
3	A	900	AMP	N3-C2-N1	-4.44	125.00	128.71
3	A	900	AMP	C8-N9-C4	-3.70	104.07	106.90
4	A	902	ADE	N9-C4-N3	-3.52	119.09	125.34
4	A	902	ADE	N6-C6-N1	3.30	125.85	119.36
3	A	900	AMP	N6-C6-N1	2.91	125.09	119.36
3	A	900	AMP	C2'-C3'-C4'	-2.80	97.07	102.65
4	A	902	ADE	N9-C8-N7	2.56	117.56	111.66
3	A	900	AMP	C2-N1-C6	2.44	123.18	118.77
4	A	902	ADE	C2-N1-C6	2.30	122.92	118.77
4	A	902	ADE	C5-C4-N3	2.26	129.22	125.94

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	821/842 (97%)	-0.21	17 (2%) 60 70	6, 15, 32, 68	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	557	ILE	5.6
1	A	555	VAL	5.5
1	A	556	HIS	4.6
1	A	21	VAL	4.1
1	A	547	ALA	3.5
1	A	558	ASN	3.3
1	A	595	ASN	3.1
1	A	560	ASN	2.9
1	A	548	TYR	2.9
1	A	550	GLU	2.9
1	A	3	PRO	2.8
1	A	549	LEU	2.7
1	A	23	ASN	2.7
1	A	319	ARG	2.6
1	A	7	GLN	2.6
1	A	554	LYS	2.3
1	A	551	ARG	2.2

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

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	LLP	A	680	24/25	0.14	0.51	8,11,21,24	0
1	SEP	A	14	10/11	0.15	0.27	20,22,23,24	0

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	ADE	A	902	10/10	0.15	6.79	28,30,32,33	0
2	GLC	A	901	12/12	0.12	0.20	7,9,11,12	0
3	AMP	A	900	23/23	0.10	-0.45	11,14,18,20	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.