Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 07:48 PM EDT

PDB ID	:	4IW2
Title	:	HSA-glucose complex
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Deposited on	:	2013-01-23
Resolution	:	2.41 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

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 2.41 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	Percentile Ranks	Value
Rfree		0.304
Clashscore		12
Ramachandran outliers		2.1%
Sidechain outliers		9.2%
RSRZ outliers		5.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

❘ Percentile relative to X-ray structures of similar resolution
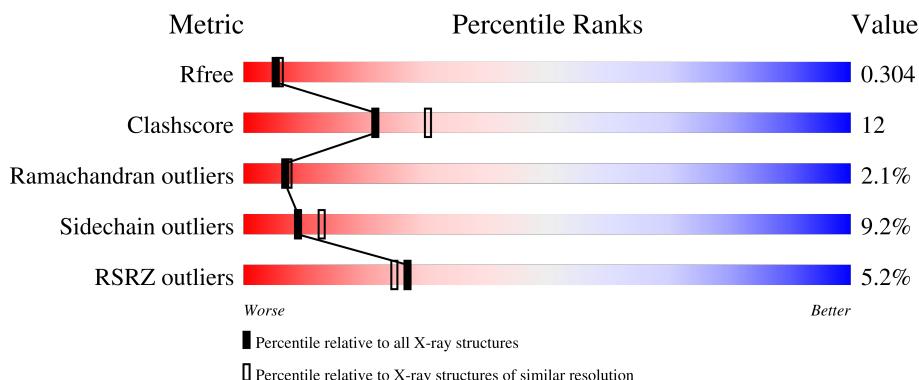
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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	585	5% / 70% / 25% / · ··
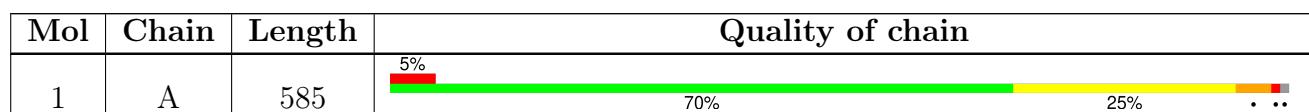
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLO	A	601	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4613 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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total 4579	C 2889	N 772	O 877	S 41	0	0	0

- Molecule 2 is D-glucose (three-letter code: GLO) (formula: $C_6H_{12}O_6$).
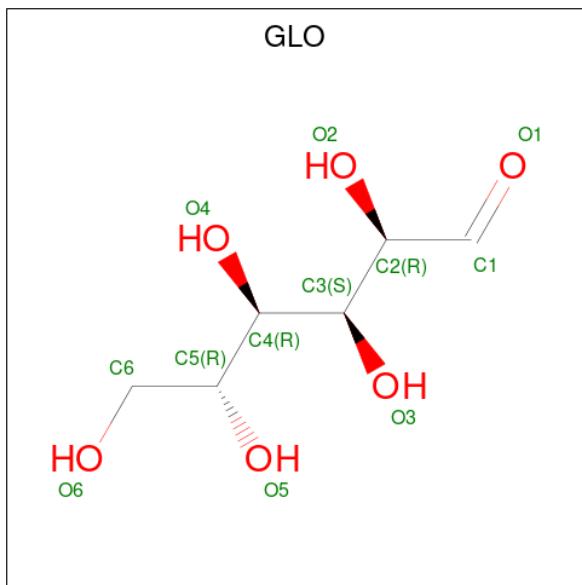
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 11	C 6	O 5	0	0

- Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).
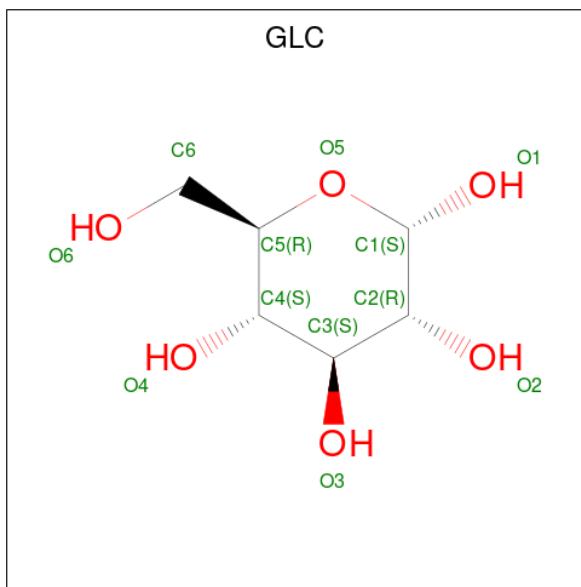
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 12	C 6	O 6	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
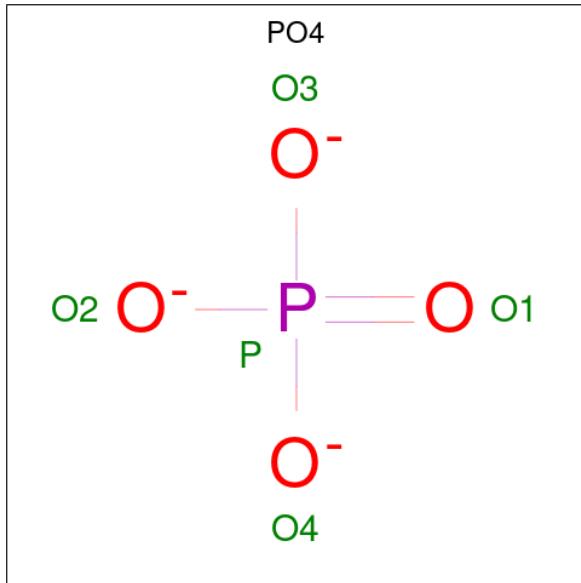
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Serum albumin
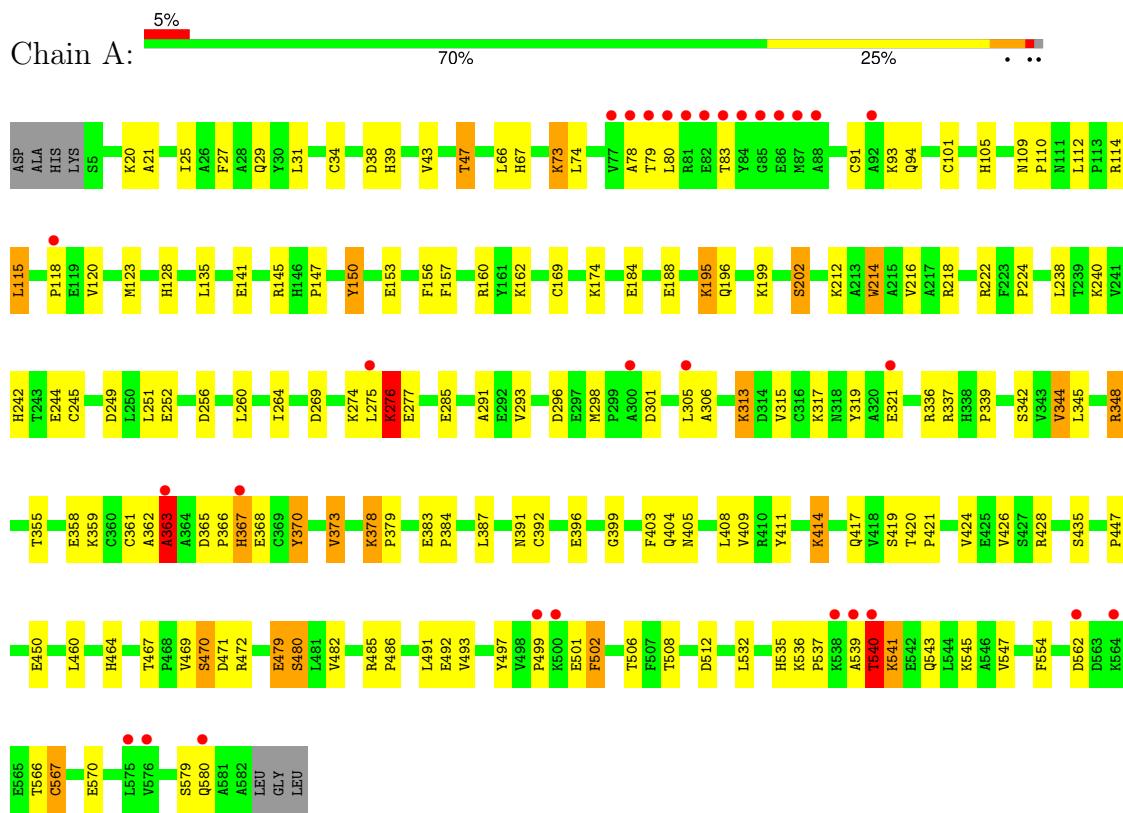
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.15Å　87.06Å　58.53Å 90.00°　102.57°　90.00°	Depositor
Resolution (Å)	33.40　–　2.41 43.53　–　2.41	Depositor EDS
% Data completeness (in resolution range)	88.3 (33.40-2.41) 96.4 (43.53-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.39Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.242　,　0.307 0.249　,　0.304	Depositor DCC
R_{free} test set	1074 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.2	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4613	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GLC, GLO, 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	0.68	1/4668 (0.0%)	0.85	3/6303 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	TRP	CD2-CE2	5.54	1.48	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	348	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	567	CYS	CA-CB-SG	5.80	124.43	114.00
1	A	363	ALA	N-CA-C	5.39	125.57	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4579	0	4467	107	0
2	A	11	0	11	7	0
3	A	12	0	12	4	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	0	1	0
All	All	4613	0	4490	108	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 12.

All (108) 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:A:539:ALA:O	1:A:540:THR:HG23	1.77	0.84
1:A:195:LYS:HE3	2:A:601:GLO:O4	1.82	0.80
1:A:502:PHE:HA	1:A:535:HIS:CE1	2.18	0.79
1:A:202:SER:HG	1:A:214:TRP:HZ3	1.30	0.77
1:A:501:GLU:O	1:A:502:PHE:HB2	1.84	0.77
1:A:260:LEU:O	1:A:264:ILE:HG13	1.90	0.71
1:A:424:VAL:O	1:A:428:ARG:HG3	1.91	0.71
1:A:547:VAL:HG13	1:A:579:SER:HB2	1.72	0.70
1:A:276:LYS:HG3	1:A:277:GLU:H	1.56	0.69
1:A:541:LYS:HB2	1:A:543:GLN:HE21	1.58	0.67
1:A:543:GLN:O	1:A:547:VAL:HG23	1.96	0.65
1:A:426:VAL:HG21	1:A:460:LEU:HB2	1.79	0.64
1:A:202:SER:OG	1:A:214:TRP:HZ3	1.82	0.63
1:A:276:LYS:HG3	1:A:277:GLU:N	2.14	0.62
1:A:34:CYS:HB3	1:A:39:HIS:NE2	2.14	0.62
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.82	0.61
2:A:601:GLO:O6	2:A:601:GLO:H2	2.01	0.61
1:A:118:PRO:HG2	1:A:123:MET:HG3	1.84	0.60
1:A:404:GLN:HG2	1:A:428:ARG:HA	1.85	0.59
1:A:195:LYS:CE	2:A:601:GLO:O4	2.50	0.59
1:A:67:HIS:CE1	1:A:249:ASP:OD1	2.56	0.58
1:A:238:LEU:HD11	3:A:602:GLC:H5	1.85	0.58
1:A:135:LEU:HD11	1:A:162:LYS:HD2	1.85	0.58
1:A:370:TYR:O	1:A:373:VAL:CG2	2.53	0.56
1:A:195:LYS:HE3	2:A:601:GLO:H62	1.87	0.56
1:A:153:GLU:O	1:A:157:PHE:HD1	1.88	0.56
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.71	0.55
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.06	0.55
1:A:365:ASP:O	1:A:366:PRO:C	2.44	0.54
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.89	0.54
1:A:27:PHE:HD1	1:A:74:LEU:HD21	1.73	0.54
1:A:536:LYS:O	1:A:540:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLN:HB3	1:A:469:VAL:HG12	1.89	0.53
1:A:464:HIS:HE1	1:A:470:SER:H	1.54	0.53
1:A:291:ALA:HB2	3:A:602:GLC:H4	1.92	0.52
1:A:366:PRO:C	1:A:368:GLU:H	2.13	0.52
1:A:305:LEU:HG	1:A:337:ARG:NH1	2.25	0.52
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.30	0.52
1:A:366:PRO:O	1:A:368:GLU:N	2.43	0.52
1:A:345:LEU:O	1:A:348:ARG:HB2	2.10	0.52
1:A:370:TYR:O	1:A:373:VAL:HG23	2.10	0.52
1:A:128:HIS:HE1	1:A:169:CYS:HB3	1.75	0.51
1:A:128:HIS:CE1	1:A:169:CYS:HB3	2.46	0.51
1:A:305:LEU:HG	1:A:337:ARG:HH11	1.76	0.51
1:A:361:CYS:C	1:A:363:ALA:H	2.13	0.51
1:A:408:LEU:HD21	1:A:424:VAL:HA	1.94	0.51
1:A:141:GLU:OE1	1:A:145:ARG:NH1	2.35	0.50
1:A:405:ASN:HA	1:A:408:LEU:HD12	1.94	0.50
1:A:196:GLN:HE22	1:A:242:HIS:CE1	2.28	0.50
1:A:355:THR:O	1:A:358:GLU:HB2	2.12	0.49
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.93	0.49
1:A:101:CYS:O	1:A:105:HIS:ND1	2.46	0.49
1:A:120:VAL:HG11	1:A:174:LYS:HB3	1.93	0.49
1:A:370:TYR:C	1:A:370:TYR:CD1	2.87	0.48
1:A:420:THR:HB	1:A:421:PRO:CD	2.43	0.48
1:A:414:LYS:HD2	1:A:491:LEU:O	2.13	0.48
1:A:313:LYS:HA	1:A:367:HIS:CE1	2.48	0.47
1:A:66:LEU:HD13	1:A:251:LEU:HD12	1.95	0.47
1:A:298:MET:HE1	1:A:339:PRO:HD3	1.97	0.47
1:A:317:LYS:O	1:A:321:GLU:HB2	2.15	0.47
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.97	0.47
1:A:240:LYS:O	1:A:244:GLU:HG3	2.15	0.47
1:A:464:HIS:CE1	1:A:469:VAL:H	2.32	0.46
1:A:497:TYR:O	1:A:499:PRO:HD3	2.16	0.46
1:A:196:GLN:HE22	1:A:242:HIS:HE1	1.62	0.46
1:A:73:LYS:HD3	1:A:73:LYS:HA	1.59	0.46
1:A:135:LEU:HD21	1:A:162:LYS:HB2	1.98	0.46
1:A:222:ARG:HD3	1:A:293:VAL:O	2.16	0.45
1:A:156:PHE:CE1	1:A:285:GLU:HG3	2.51	0.45
1:A:128:HIS:CE1	1:A:169:CYS:CB	3.00	0.45
1:A:411:TYR:HA	1:A:414:LYS:HB2	1.98	0.45
1:A:27:PHE:HD1	1:A:74:LEU:CD2	2.31	0.44
1:A:160:ARG:NH2	1:A:188:GLU:OE2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LYS:HA	1:A:367:HIS:NE2	2.33	0.44
1:A:342:SER:HA	1:A:447:PRO:HA	1.99	0.44
1:A:566:THR:O	1:A:570:GLU:HG2	2.17	0.44
1:A:78:ALA:HB3	1:A:91:CYS:SG	2.58	0.44
1:A:244:GLU:OE1	1:A:256:ASP:OD2	2.36	0.44
1:A:387:LEU:HG	1:A:391:ASN:ND2	2.33	0.43
1:A:399:GLY:O	1:A:403:PHE:HB2	2.18	0.43
1:A:547:VAL:CG1	1:A:579:SER:HB2	2.45	0.43
1:A:212:LYS:O	1:A:216:VAL:HG23	2.19	0.43
1:A:378:LYS:CB	1:A:379:PRO:HD3	2.46	0.43
1:A:39:HIS:O	1:A:43:VAL:HG23	2.19	0.43
1:A:238:LEU:CD1	3:A:602:GLC:H5	2.48	0.43
1:A:150:TYR:OH	3:A:602:GLC:O4	2.37	0.43
1:A:110:PRO:O	1:A:112:LEU:N	2.52	0.42
1:A:405:ASN:O	1:A:409:VAL:HG23	2.19	0.42
1:A:319:TYR:OH	1:A:358:GLU:HG2	2.19	0.42
1:A:301:ASP:OD2	1:A:301:ASP:C	2.58	0.42
1:A:195:LYS:NZ	2:A:601:GLO:O4	2.52	0.42
1:A:29:GLN:HG2	1:A:147:PRO:HA	2.00	0.42
1:A:43:VAL:O	1:A:47:THR:OG1	2.36	0.42
1:A:115:LEU:HD13	1:A:145:ARG:NH2	2.35	0.42
1:A:21:ALA:O	1:A:25:ILE:HG13	2.20	0.41
1:A:218:ARG:NE	2:A:601:GLO:O3	2.52	0.41
1:A:370:TYR:O	1:A:373:VAL:HG22	2.20	0.41
1:A:450:GLU:OE2	1:A:485:ARG:NE	2.38	0.41
1:A:313:LYS:C	1:A:315:VAL:H	2.24	0.41
1:A:344:VAL:HG21	1:A:450:GLU:HG2	2.03	0.41
1:A:366:PRO:C	1:A:368:GLU:N	2.74	0.41
1:A:195:LYS:CE	2:A:601:GLO:H62	2.50	0.40
1:A:275:LEU:O	1:A:276:LYS:C	2.60	0.40
1:A:348:ARG:HG3	1:A:482:VAL:CG1	2.51	0.40
1:A:479:GLU:O	1:A:480:SER:CB	2.68	0.40
1:A:392:CYS:O	1:A:396:GLU:HG2	2.20	0.40
1:A:199:LYS:NZ	5:A:704:HOH:O	2.55	0.40
1:A:464:HIS:CE1	1:A:470:SER:H	2.37	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	576/585 (98%)	527 (92%)	37 (6%)	12 (2%)	7 7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ALA
1	A	480	SER
1	A	502	PHE
1	A	540	THR
1	A	541	LYS
1	A	276	LYS
1	A	306	ALA
1	A	562	ASP
1	A	367	HIS
1	A	150	TYR
1	A	362	ALA
1	A	537	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	501/511 (98%)	455 (91%)	46 (9%)	9 13

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	31	LEU
1	A	38	ASP
1	A	47	THR
1	A	73	LYS
1	A	79	THR
1	A	80	LEU
1	A	83	THR
1	A	93	LYS
1	A	94	GLN
1	A	109	ASN
1	A	114	ARG
1	A	115	LEU
1	A	184	GLU
1	A	195	LYS
1	A	202	SER
1	A	245	CYS
1	A	269	ASP
1	A	274	LYS
1	A	276	LYS
1	A	313	LYS
1	A	336	ARG
1	A	344	VAL
1	A	359	LYS
1	A	370	TYR
1	A	373	VAL
1	A	378	LYS
1	A	414	LYS
1	A	419	SER
1	A	435	SER
1	A	467	THR
1	A	470	SER
1	A	471	ASP
1	A	472	ARG
1	A	479	GLU
1	A	492	GLU
1	A	493	VAL
1	A	506	THR
1	A	508	THR
1	A	512	ASP
1	A	532	LEU
1	A	540	THR
1	A	545	LYS

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Mol	Chain	Res	Type
1	A	554	PHE
1	A	567	CYS
1	A	580	GLN

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	67	HIS
1	A	109	ASN
1	A	128	HIS
1	A	196	GLN
1	A	385	GLN
1	A	386	ASN
1	A	464	HIS
1	A	483	ASN
1	A	535	HIS
1	A	543	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	GLC	A	602	-	12,12,12	0.81	0	17,17,17	1.96	6 (35%)
2	GLO	A	601	1	10,10,11	0.36	0	13,13,14	0.83	0
4	PO4	A	603	-	4,4,4	0.74	0	6,6,6	1.33	1 (16%)

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	GLC	A	602	-	-	2/2/22/22	0/1/1/1
2	GLO	A	601	1	-	11/14/14/16	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	GLC	O5-C5-C6	3.73	115.67	106.44
3	A	602	GLC	C1-C2-C3	3.63	117.76	110.36
3	A	602	GLC	O2-C2-C3	-2.85	103.66	110.38
4	A	603	PO4	O2-P-O1	-2.69	101.45	110.95
3	A	602	GLC	O2-C2-C1	-2.60	103.24	109.25
3	A	602	GLC	C3-C4-C5	-2.40	105.89	110.23
3	A	602	GLC	O4-C4-C5	-2.15	104.02	109.32

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GLO	O2-C2-C3-O3
2	A	601	GLO	C1-C2-C3-O3
2	A	601	GLO	O4-C4-C5-O5
2	A	601	GLO	O4-C4-C5-C6
2	A	601	GLO	O5-C5-C6-O6
2	A	601	GLO	C3-C4-C5-C6
2	A	601	GLO	C3-C4-C5-O5
3	A	602	GLC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	601	GLO	O2-C2-C3-C4
2	A	601	GLO	C2-C3-C4-C5
2	A	601	GLO	C4-C5-C6-O6
2	A	601	GLO	C1-C2-C3-C4
3	A	602	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	GLC	4	0
2	A	601	GLO	7	0

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	578/585 (98%)	0.27	30 (5%)	27	25	34, 53, 91, 153	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ALA	8.4
1	A	84	TYR	7.5
1	A	79	THR	7.2
1	A	83	THR	7.0
1	A	85	GLY	6.3
1	A	80	LEU	6.0
1	A	87	MET	5.7
1	A	81	ARG	4.9
1	A	575	LEU	4.8
1	A	82	GLU	4.8
1	A	77	VAL	4.2
1	A	321	GLU	3.9
1	A	300	ALA	3.7
1	A	564	LYS	3.6
1	A	305	LEU	3.5
1	A	539	ALA	3.2
1	A	576	VAL	3.2
1	A	88	ALA	3.2
1	A	363	ALA	2.7
1	A	86	GLU	2.7
1	A	538	LYS	2.5
1	A	499	PRO	2.4
1	A	580	GLN	2.3
1	A	275	LEU	2.2
1	A	500	LYS	2.2
1	A	562	ASP	2.1
1	A	367	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	540	THR	2.1
1	A	118	PRO	2.0
1	A	92	ALA	2.0

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 monosaccharides 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. 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	GLO	A	601	11/12	0.79	0.17	74,76,79,85	0
3	GLC	A	602	12/12	0.84	0.33	51,57,61,62	0
4	PO4	A	603	5/5	0.94	0.27	86,88,91,93	0

6.5 Other polymers ⓘ

There are no such residues in this entry.