



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:56 PM UTC

PDB ID : 1FA9 / pdb_00001fa9
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH AMP
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Deposited on : 2000-07-12
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

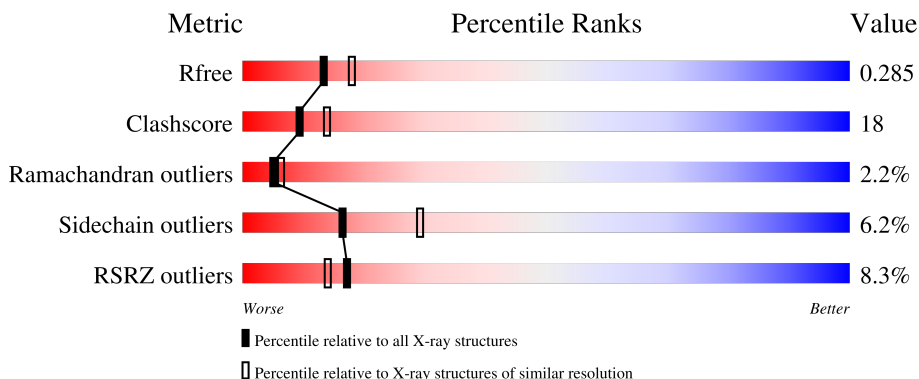
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	846	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7042 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.

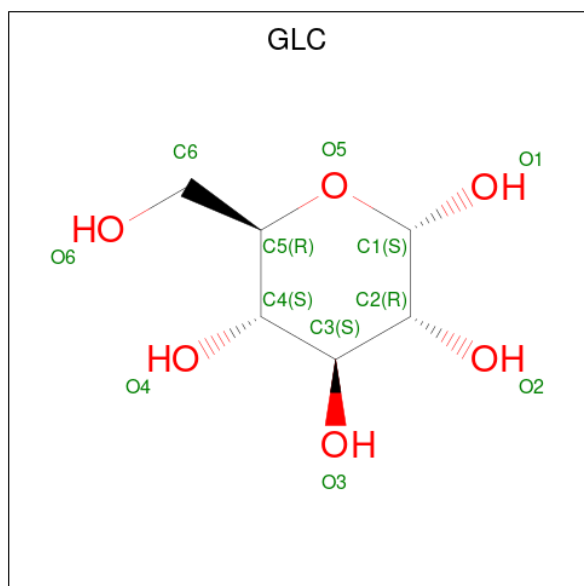
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE, LIVER FORM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	834	6750	4325	1154	1241	1	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

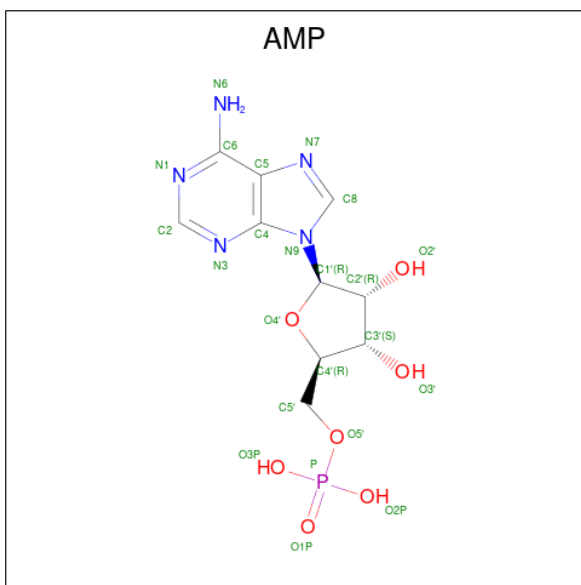
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SEP	SER	modified residue	UNP P06737

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



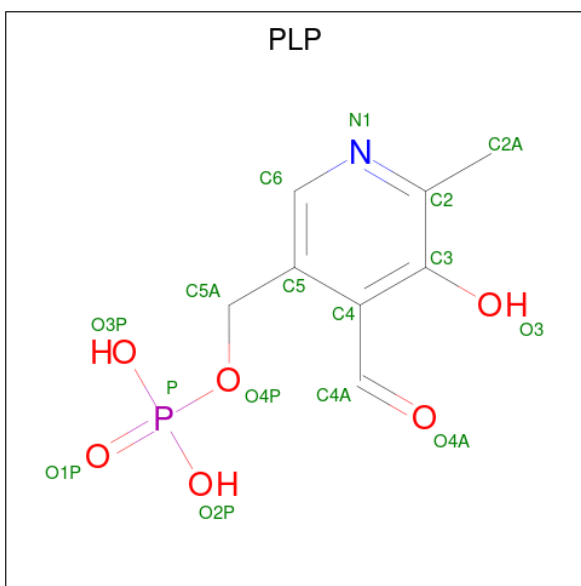
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

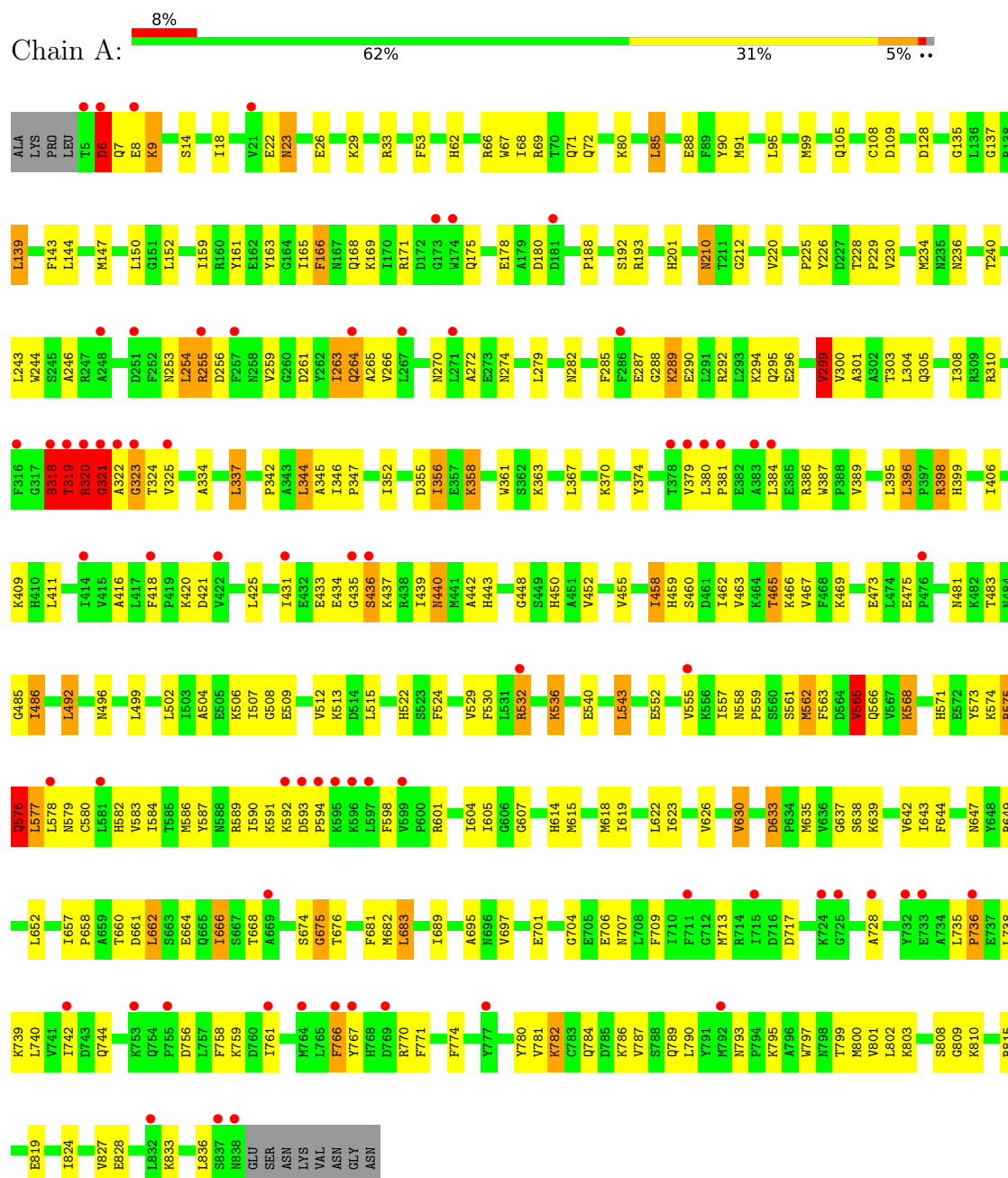
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total 242	O 242	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: GLYCOGEN PHOSPHORYLASE, LIVER FORM



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.91Å 123.91Å 127.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 97.7 (50.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.235 , 0.295 0.206 , 0.285	Depositor DCC
R_{free} test set	4609 reflections (8.79%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.76	6/6887 (0.1%)	1.15	37/9311 (0.4%)

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	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	GLY	C-N	-41.58	0.75	1.33
1	A	318	SER	C-N	27.60	1.72	1.33
1	A	320	ARG	C-N	-9.54	1.19	1.33
1	A	319	THR	C-N	-9.49	1.16	1.33
1	A	321	GLY	N-CA	-6.51	1.35	1.45
1	A	319	THR	CA-C	-5.70	1.45	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	SER	O-C-N	-51.54	54.04	122.59
1	A	321	GLY	O-C-N	18.72	147.03	122.70
1	A	320	ARG	O-C-N	14.33	141.63	123.01
1	A	319	THR	O-C-N	11.58	138.00	122.59
1	A	321	GLY	N-CA-C	-10.90	87.35	113.18
1	A	577	LEU	N-CA-C	-8.04	101.80	111.69
1	A	467	VAL	N-CA-C	7.60	117.71	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ARG	CA-C-N	6.95	135.03	121.41
1	A	320	ARG	C-N-CA	6.95	135.03	121.41
1	A	824	ILE	N-CA-C	6.56	116.80	111.62
1	A	299	VAL	CB-CA-C	-6.25	103.70	112.14
1	A	475	GLU	CA-C-N	6.18	125.67	119.24
1	A	475	GLU	C-N-CA	6.18	125.67	119.24
1	A	319	THR	CB-CA-C	-5.91	98.66	110.42
1	A	767	TYR	N-CA-C	5.84	119.88	112.87
1	A	91	MET	N-CA-C	5.78	119.51	112.23
1	A	356	ILE	N-CA-C	5.64	116.29	110.82
1	A	562	MET	N-CA-C	5.48	117.06	111.14
1	A	793	ASN	CA-C-N	5.45	124.91	119.24
1	A	793	ASN	C-N-CA	5.45	124.91	119.24
1	A	565	VAL	N-CA-C	5.43	117.22	108.85
1	A	139	LEU	N-CA-C	-5.38	105.33	111.14
1	A	212	GLY	N-CA-C	5.35	118.27	111.85
1	A	406	ILE	N-CA-C	-5.32	105.53	110.53
1	A	321	GLY	CA-C-N	-5.28	111.45	121.54
1	A	321	GLY	C-N-CA	-5.28	111.45	121.54
1	A	9	LYS	N-CA-C	-5.27	105.59	112.23
1	A	234	MET	N-CA-C	5.25	118.83	111.90
1	A	532	ARG	N-CA-C	-5.17	105.56	111.14
1	A	263	ILE	N-CA-C	-5.15	106.66	111.45
1	A	416	ALA	N-CA-C	-5.11	107.20	112.93
1	A	666	ILE	N-CA-C	5.04	119.82	109.34
1	A	240	THR	N-CA-C	5.03	117.10	108.90
1	A	465	THR	N-CA-C	5.03	119.28	112.04
1	A	633	ASP	CA-C-N	5.01	124.79	119.28
1	A	633	ASP	C-N-CA	5.01	124.79	119.28
1	A	507	ILE	N-CA-C	5.00	117.18	111.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ARG	Mainchain

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	6750	0	6734	242	1
2	A	12	0	12	5	0
3	A	23	0	12	1	0
4	A	15	0	7	2	0
5	A	242	0	0	9	0
All	All	7042	0	6765	244	1

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 18.

All (244) 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:320:ARG:NH1	1:A:323:GLY:HA2	1.33	1.36
1:A:318:SER:O	1:A:319:THR:OG1	1.56	1.18
1:A:320:ARG:NH1	1:A:323:GLY:CA	2.15	1.08
1:A:486:ILE:HD11	1:A:676:THR:HG23	1.38	1.03
1:A:320:ARG:HH11	1:A:323:GLY:HA2	1.13	0.96
1:A:320:ARG:HH11	1:A:323:GLY:CA	1.81	0.90
1:A:320:ARG:CZ	1:A:323:GLY:HA2	2.04	0.87
1:A:69:ARG:HH11	1:A:72:GLN:HE22	1.19	0.84
1:A:23:ASN:H	1:A:23:ASN:HD22	1.28	0.82
1:A:455:VAL:H	1:A:459:HIS:HD2	1.27	0.82
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.63	0.81
1:A:319:THR:O	1:A:322:ALA:HB3	1.79	0.81
1:A:440:ASN:HD22	1:A:443:HIS:H	1.32	0.77
1:A:99:MET:HE3	1:A:108:CYS:HB2	1.70	0.74
1:A:758:PHE:O	1:A:761:ILE:HG22	1.88	0.73
1:A:69:ARG:NH1	1:A:72:GLN:HE22	1.86	0.72
1:A:384:LEU:HB2	1:A:386:ARG:HH21	1.54	0.71
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.73	0.70
1:A:319:THR:HG22	1:A:320:ARG:H	1.55	0.70
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.72	0.70
1:A:22:GLU:HA	5:A:2184:HOH:O	1.90	0.70
1:A:462:ILE:HA	1:A:466:LYS:HD3	1.74	0.70
1:A:455:VAL:H	1:A:459:HIS:CD2	2.10	0.68
1:A:318:SER:C	1:A:319:THR:OG1	2.37	0.67
1:A:575:ARG:C	1:A:577:LEU:H	2.02	0.67
1:A:69:ARG:HH11	1:A:72:GLN:NE2	1.91	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLY:O	1:A:323:GLY:N	2.28	0.66
1:A:668:THR:OG1	1:A:771:PHE:HB3	1.97	0.65
1:A:676:THR:HB	2:A:998:GLC:H62	1.79	0.65
1:A:7:GLN:HG3	1:A:8:GLU:H	1.61	0.65
1:A:571:HIS:H	1:A:576:GLN:HE22	1.43	0.64
1:A:152:LEU:HD22	1:A:827:VAL:CG1	2.29	0.63
1:A:579:ASN:O	1:A:583:VAL:HG23	1.98	0.63
1:A:440:ASN:ND2	1:A:443:HIS:H	1.97	0.63
1:A:529:VAL:O	1:A:532:ARG:HB3	1.99	0.62
1:A:261:ASP:HB3	1:A:264:GLN:HB2	1.79	0.62
1:A:676:THR:HG21	5:A:2028:HOH:O	2.00	0.62
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.82	0.62
1:A:319:THR:CG2	1:A:320:ARG:H	2.11	0.62
1:A:455:VAL:O	1:A:483:THR:HA	1.99	0.62
1:A:370:LYS:NZ	1:A:370:LYS:HB3	2.15	0.61
1:A:575:ARG:O	1:A:576:GLN:HG2	2.01	0.61
1:A:358:LYS:HE3	5:A:2053:HOH:O	1.99	0.61
1:A:492:LEU:HG	1:A:683:LEU:HD22	1.82	0.61
1:A:318:SER:HA	1:A:325:VAL:CG1	2.30	0.60
1:A:728:ALA:HB1	1:A:774:PHE:HD1	1.65	0.60
1:A:571:HIS:H	1:A:576:GLN:NE2	2.00	0.60
1:A:455:VAL:N	1:A:459:HIS:HD2	1.99	0.60
1:A:396:LEU:HB3	1:A:399:HIS:HB2	1.83	0.60
1:A:135:GLY:HA3	2:A:998:GLC:O5	2.02	0.60
1:A:7:GLN:HG3	1:A:8:GLU:N	2.17	0.59
1:A:266:VAL:HG12	1:A:266:VAL:O	2.01	0.59
1:A:562:MET:O	1:A:563:PHE:HB2	2.03	0.59
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.84	0.59
1:A:210:ASN:N	1:A:210:ASN:HD22	2.00	0.59
1:A:270:ASN:HB2	5:A:2220:HOH:O	2.02	0.59
1:A:411:LEU:HD22	1:A:425:LEU:HD22	1.84	0.59
1:A:562:MET:O	1:A:661:ASP:HB2	2.03	0.59
1:A:568:LYS:NZ	1:A:568:LYS:HB3	2.18	0.58
1:A:152:LEU:HD22	1:A:827:VAL:HG12	1.85	0.58
1:A:728:ALA:HB1	1:A:774:PHE:CD1	2.39	0.58
1:A:450:HIS:HE1	5:A:2092:HOH:O	1.86	0.57
1:A:7:GLN:HG2	1:A:9:LYS:HD3	1.86	0.57
1:A:568:LYS:O	1:A:607:GLY:HA3	2.03	0.57
1:A:352:ILE:HA	1:A:356:ILE:HD12	1.86	0.57
2:A:998:GLC:H61	4:A:999:PLP:P	2.45	0.57
1:A:23:ASN:HD22	1:A:23:ASN:N	1.96	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:SER:HA	1:A:325:VAL:HG11	1.85	0.56
1:A:320:ARG:HH11	1:A:323:GLY:C	2.12	0.56
1:A:321:GLY:C	1:A:323:GLY:N	2.62	0.56
1:A:384:LEU:HB2	1:A:386:ARG:NH2	2.19	0.56
1:A:254:LEU:HD13	1:A:255:ARG:HH22	1.71	0.56
1:A:674:SER:HB3	2:A:998:GLC:O4	2.06	0.56
1:A:728:ALA:HB3	1:A:766:PHE:HA	1.87	0.55
1:A:799:THR:HB	5:A:2231:HOH:O	2.05	0.55
1:A:790:LEU:HG	1:A:797:TRP:HE3	1.72	0.55
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.88	0.54
2:A:998:GLC:H61	4:A:999:PLP:O2P	2.08	0.54
1:A:532:ARG:NH1	1:A:536:LYS:HG3	2.21	0.54
1:A:344:LEU:HB2	5:A:2197:HOH:O	2.08	0.54
1:A:7:GLN:HG3	1:A:9:LYS:H	1.72	0.54
1:A:558:ASN:HB3	1:A:561:SER:HB2	1.90	0.54
1:A:582:HIS:HD2	1:A:781:VAL:HG13	1.73	0.54
1:A:614:HIS:O	1:A:618:MET:HG2	2.08	0.54
1:A:292:ARG:O	1:A:296:GLU:HG3	2.08	0.53
1:A:88:GLU:HG2	1:A:137:GLY:HA3	1.91	0.53
1:A:458:ILE:O	1:A:462:ILE:HG13	2.08	0.53
1:A:322:ALA:O	1:A:324:THR:N	2.41	0.53
1:A:68:ILE:O	1:A:72:GLN:HG3	2.08	0.53
1:A:622:LEU:O	1:A:626:VAL:HG23	2.09	0.53
1:A:165:ILE:O	1:A:166:PHE:HB3	2.09	0.53
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.91	0.53
1:A:355:ASP:OD1	1:A:398:ARG:HD3	2.08	0.53
1:A:586:MET:O	1:A:590:ILE:HG13	2.09	0.53
1:A:67:TRP:O	1:A:71:GLN:HG2	2.09	0.52
1:A:530:PHE:HE2	1:A:802:LEU:HD13	1.74	0.52
1:A:662:LEU:HD21	1:A:689:ILE:HB	1.91	0.52
1:A:358:LYS:HB2	1:A:358:LYS:NZ	2.24	0.52
1:A:689:ILE:HG23	1:A:689:ILE:O	2.09	0.52
1:A:263:ILE:HD12	1:A:263:ILE:N	2.24	0.52
1:A:321:GLY:C	1:A:323:GLY:H	2.16	0.52
1:A:707:ASN:ND2	1:A:803:LYS:HD3	2.25	0.52
1:A:380:LEU:HD12	1:A:381:PRO:HD2	1.92	0.52
1:A:522:HIS:C	1:A:524:PHE:H	2.17	0.52
1:A:697:VAL:O	1:A:701:GLU:HG3	2.10	0.52
1:A:509:GLU:O	1:A:512:VAL:HG22	2.10	0.51
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.45	0.51
1:A:370:LYS:HB3	1:A:370:LYS:HZ3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ILE:HB	1:A:347:PRO:HD3	1.91	0.51
1:A:53:PHE:CE1	1:A:188:PRO:HD3	2.46	0.51
1:A:626:VAL:O	1:A:630:VAL:HG13	2.11	0.51
1:A:418:PHE:HB3	1:A:421:ASP:CB	2.41	0.51
1:A:22:GLU:HB3	1:A:62:HIS:CE1	2.45	0.50
1:A:469:LYS:O	1:A:473:GLU:HG3	2.11	0.50
1:A:738:LEU:HD11	1:A:774:PHE:CD2	2.46	0.50
1:A:304:LEU:O	1:A:308:ILE:HG12	2.11	0.50
1:A:565:VAL:HG11	1:A:660:THR:HG22	1.93	0.50
1:A:582:HIS:CD2	1:A:781:VAL:HG13	2.46	0.50
1:A:295:GLN:O	1:A:299:VAL:HG23	2.11	0.50
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.94	0.50
1:A:782:LYS:HE3	1:A:782:LYS:HA	1.94	0.50
1:A:810:LYS:O	1:A:815:ARG:NH1	2.41	0.49
1:A:660:THR:HG21	1:A:681:PHE:HE1	1.76	0.49
1:A:459:HIS:O	1:A:463:VAL:HG23	2.13	0.49
1:A:578:LEU:HG	1:A:780:TYR:CD2	2.48	0.49
1:A:289:LYS:HG2	1:A:387:TRP:HZ3	1.78	0.49
1:A:418:PHE:HB3	1:A:421:ASP:HB3	1.94	0.49
1:A:159:ILE:HD11	1:A:299:VAL:HG22	1.95	0.49
1:A:598:PHE:CD2	1:A:639:LYS:HG2	2.47	0.49
1:A:210:ASN:N	1:A:210:ASN:ND2	2.59	0.49
1:A:433:GLU:HG3	1:A:437:LYS:HE2	1.94	0.49
1:A:6:ASP:O	1:A:7:GLN:HB3	2.13	0.48
1:A:675:GLY:N	1:A:695:ALA:HB2	2.28	0.48
1:A:504:ALA:HA	1:A:508:GLY:O	2.14	0.48
1:A:557:ILE:O	1:A:559:PRO:HD3	2.14	0.48
1:A:99:MET:HE2	1:A:105:GLN:HA	1.96	0.48
1:A:431:ILE:HD11	1:A:437:LYS:HD3	1.94	0.48
1:A:605:ILE:O	1:A:644:PHE:HA	2.13	0.48
1:A:815:ARG:O	1:A:819:GLU:HG3	2.14	0.48
1:A:23:ASN:HD21	1:A:26:GLU:HG2	1.79	0.48
1:A:485:GLY:O	1:A:486:ILE:HD12	2.14	0.48
1:A:575:ARG:O	1:A:577:LEU:N	2.47	0.48
1:A:255:ARG:O	1:A:259:VAL:HG23	2.14	0.47
1:A:386:ARG:HG3	1:A:386:ARG:HH11	1.78	0.47
1:A:236:ASN:ND2	1:A:833:LYS:HE2	2.29	0.47
1:A:742:ILE:HD11	1:A:774:PHE:HE2	1.79	0.47
1:A:637:GLY:C	1:A:639:LYS:H	2.22	0.47
1:A:801:VAL:HG11	5:A:2159:HOH:O	2.13	0.47
1:A:192:SER:HB3	1:A:226:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:C	1:A:436:SER:H	2.23	0.47
1:A:492:LEU:HG	1:A:683:LEU:CD2	2.43	0.47
1:A:573:TYR:CZ	1:A:574:LYS:HE2	2.50	0.47
1:A:23:ASN:H	1:A:23:ASN:ND2	2.05	0.47
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.80	0.46
1:A:633:ASP:OD2	1:A:635:MET:HB2	2.15	0.46
1:A:279:LEU:HD12	5:A:2080:HOH:O	2.15	0.46
1:A:344:LEU:O	1:A:347:PRO:HD2	2.16	0.46
1:A:168:GLN:O	1:A:647:ASN:HB2	2.16	0.46
1:A:290:GLU:O	1:A:294:LYS:HG3	2.15	0.46
1:A:440:ASN:HD21	1:A:442:ALA:HB3	1.81	0.46
1:A:515:LEU:HB3	1:A:809:GLY:O	2.16	0.46
1:A:555:VAL:HG11	1:A:643:ILE:HD11	1.98	0.46
1:A:587:TYR:O	1:A:591:LYS:HG2	2.16	0.46
1:A:386:ARG:HD3	1:A:440:ASN:HA	1.98	0.46
1:A:282:ASN:O	1:A:288:GLY:HA3	2.16	0.45
1:A:619:ILE:O	1:A:623:ILE:HG13	2.16	0.45
1:A:689:ILE:HA	1:A:709:PHE:HB2	1.97	0.45
1:A:601:ARG:HH12	1:A:784:GLN:CD	2.23	0.45
1:A:256:ASP:HB3	1:A:261:ASP:HB2	1.98	0.45
1:A:289:LYS:HB2	1:A:289:LYS:NZ	2.32	0.45
1:A:381:PRO:HA	1:A:384:LEU:HG	1.97	0.45
1:A:99:MET:CE	1:A:105:GLN:HA	2.46	0.45
1:A:483:THR:O	1:A:815:ARG:NH2	2.40	0.45
1:A:615:MET:HE2	1:A:761:ILE:HG13	1.97	0.45
1:A:460:SER:OG	1:A:481:ASN:ND2	2.37	0.45
1:A:486:ILE:CD1	1:A:676:THR:HG23	2.28	0.45
1:A:573:TYR:OH	1:A:574:LYS:HE2	2.16	0.45
1:A:386:ARG:HA	1:A:439:ILE:O	2.17	0.45
1:A:466:LYS:HD2	1:A:466:LYS:N	2.31	0.45
1:A:662:LEU:HD11	1:A:689:ILE:HG21	1.98	0.45
1:A:657:ILE:HG12	1:A:681:PHE:CE1	2.52	0.44
1:A:165:ILE:HG23	1:A:166:PHE:N	2.32	0.44
1:A:319:THR:O	1:A:325:VAL:HG13	2.15	0.44
1:A:589:ARG:O	1:A:592:LYS:HB2	2.17	0.44
1:A:300:VAL:HG13	1:A:345:ALA:HA	1.98	0.44
1:A:310:ARG:HD3	3:A:997:AMP:O3P	2.17	0.44
1:A:675:GLY:CA	1:A:695:ALA:HB2	2.48	0.44
1:A:163:TYR:O	1:A:180:ASP:HB3	2.16	0.44
1:A:575:ARG:C	1:A:577:LEU:N	2.72	0.44
1:A:682:MET:HG2	1:A:808:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LEU:HG	1:A:787:VAL:HG11	1.99	0.44
1:A:740:LEU:O	1:A:744:GLN:HG3	2.18	0.43
1:A:584:ILE:O	1:A:587:TYR:HB3	2.18	0.43
1:A:318:SER:HA	1:A:325:VAL:HG12	1.98	0.43
1:A:735:LEU:HA	1:A:736:PRO:HD3	1.84	0.43
1:A:358:LYS:HB2	1:A:358:LYS:HZ3	1.82	0.43
1:A:592:LYS:HE3	1:A:592:LYS:HB3	1.88	0.43
1:A:29:LYS:HG2	1:A:33:ARG:NH2	2.33	0.43
1:A:465:THR:OG1	1:A:466:LYS:HD2	2.19	0.43
1:A:604:ILE:HA	1:A:643:ILE:O	2.18	0.43
1:A:236:ASN:HD21	1:A:833:LYS:HE2	1.84	0.43
1:A:266:VAL:O	1:A:266:VAL:CG1	2.65	0.43
1:A:143:PHE:O	1:A:147:MET:HG3	2.19	0.43
1:A:756:ASP:O	1:A:759:LYS:HB2	2.18	0.42
1:A:795:LYS:O	1:A:799:THR:HG23	2.19	0.42
1:A:228:THR:HA	1:A:229:PRO:HD3	1.87	0.42
1:A:319:THR:C	1:A:322:ALA:HB3	2.44	0.42
1:A:361:TRP:CZ3	1:A:409:LYS:HD2	2.54	0.42
1:A:800:MET:O	1:A:803:LYS:HB2	2.19	0.42
1:A:707:ASN:HD21	1:A:803:LYS:HD3	1.84	0.42
1:A:7:GLN:CG	1:A:8:GLU:H	2.32	0.42
1:A:285:PHE:CD1	1:A:287:GLU:HB2	2.54	0.42
1:A:301:ALA:O	1:A:305:GLN:HG3	2.20	0.42
1:A:389:VAL:HG12	1:A:439:ILE:CG1	2.49	0.42
1:A:66:ARG:HG2	1:A:836:LEU:HD21	2.02	0.42
1:A:363:LYS:O	1:A:367:LEU:HG	2.20	0.42
1:A:515:LEU:HG	1:A:809:GLY:HA2	2.01	0.42
1:A:169:LYS:HD2	1:A:178:GLU:CD	2.45	0.41
1:A:435:GLY:O	1:A:436:SER:HB3	2.20	0.41
1:A:615:MET:O	1:A:619:ILE:HG13	2.19	0.41
1:A:704:GLY:C	1:A:706:GLU:N	2.77	0.41
1:A:253:ASN:HB3	1:A:265:ALA:HA	2.03	0.41
1:A:320:ARG:NH1	1:A:323:GLY:C	2.76	0.41
1:A:201:HIS:CE1	1:A:220:VAL:HG22	2.55	0.41
1:A:270:ASN:ND2	1:A:274:ASN:HD21	2.18	0.41
1:A:615:MET:HE1	1:A:761:ILE:HA	2.01	0.41
1:A:379:VAL:HB	1:A:459:HIS:ND1	2.35	0.41
1:A:506:LYS:HB3	1:A:524:PHE:CZ	2.56	0.41
1:A:161:TYR:CE2	1:A:279:LEU:HD13	2.55	0.41
1:A:337:LEU:HG	1:A:342:PRO:HG2	2.02	0.41
1:A:536:LYS:O	1:A:540:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LEU:HD11	1:A:774:PHE:CE2	2.55	0.41
1:A:379:VAL:HB	1:A:459:HIS:CE1	2.56	0.41
1:A:496:ASN:ND2	1:A:658:PRO:HB3	2.35	0.40
1:A:144:LEU:HB3	1:A:230:VAL:HG11	2.04	0.40
1:A:246:ALA:HB1	1:A:272:ALA:O	2.22	0.40
1:A:580:CYS:SG	1:A:622:LEU:HD13	2.61	0.40
1:A:797:TRP:O	1:A:801:VAL:HG23	2.21	0.40
1:A:395:LEU:O	1:A:396:LEU:HD13	2.21	0.40
1:A:462:ILE:O	1:A:466:LYS:HB2	2.21	0.40
1:A:639:LYS:HE3	1:A:639:LYS:HB2	1.84	0.40
1:A:786:LYS:HA	1:A:789:GLN:HG2	2.03	0.40
1:A:374:TYR:O	1:A:452:VAL:HA	2.22	0.40
1:A:736:PRO:O	1:A:739:LYS:HB3	2.21	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:THR:CG2	1:A:543:LEU:CD2[5_665]	1.53	0.67

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	831/846 (98%)	761 (92%)	52 (6%)	18 (2%)	5 6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	SER
1	A	319	THR
1	A	436	SER

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Mol	Chain	Res	Type
1	A	166	PHE
1	A	321	GLY
1	A	323	GLY
1	A	576	GLN
1	A	575	ARG
1	A	594	PRO
1	A	638	SER
1	A	736	PRO
1	A	766	PHE
1	A	770	ARG
1	A	6	ASP
1	A	593	ASP
1	A	18	ILE
1	A	675	GLY
1	A	666	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	725/738 (98%)	680 (94%)	45 (6%)	16	29

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	23	ASN
1	A	85	LEU
1	A	90	TYR
1	A	95	LEU
1	A	109	ASP
1	A	128	ASP
1	A	139	LEU
1	A	150	LEU
1	A	171	ARG
1	A	210	ASN

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	254	LEU
1	A	255	ARG
1	A	264	GLN
1	A	289	LYS
1	A	299	VAL
1	A	318	SER
1	A	319	THR
1	A	337	LEU
1	A	344	LEU
1	A	358	LYS
1	A	396	LEU
1	A	398	ARG
1	A	420	LYS
1	A	440	ASN
1	A	458	ILE
1	A	486	ILE
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	513	LYS
1	A	536	LYS
1	A	543	LEU
1	A	552	GLU
1	A	565	VAL
1	A	568	LYS
1	A	576	GLN
1	A	630	VAL
1	A	649	ARG
1	A	652	LEU
1	A	662	LEU
1	A	683	LEU
1	A	782	LYS
1	A	828	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	23	ASN
1	A	32	ASN
1	A	62	HIS

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Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	HIS
1	A	114	GLN
1	A	167	ASN
1	A	210	ASN
1	A	219	GLN
1	A	258	ASN
1	A	270	ASN
1	A	282	ASN
1	A	369	GLN
1	A	376	ASN
1	A	399	HIS
1	A	408	GLN
1	A	410	HIS
1	A	440	ASN
1	A	459	HIS
1	A	481	ASN
1	A	517	GLN
1	A	541	ASN
1	A	547	GLN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	789	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	8,9,10	1.29	1 (12%)	7,12,14	6.76	4 (57%)

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	-	3/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	SEP	P-O2P	-2.05	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	SEP	OG-CB-CA	16.31	124.01	108.14
1	A	14	SEP	O2P-P-O1P	5.96	134.07	110.83
1	A	14	SEP	O3P-P-O1P	-3.33	97.87	110.83
1	A	14	SEP	O3P-P-O2P	-2.06	100.07	107.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	14	SEP	C-CA-CB-OG
1	A	14	SEP	CA-CB-OG-P
1	A	14	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
2	GLC	A	998	-	12,12,12	0.26	0	17,17,17	0.53	0
3	AMP	A	997	-	25,25,25	0.88	0	37,38,38	0.95	1 (2%)
4	PLP	A	999	1	15,15,16	2.51	6 (40%)	21,22,23	1.51	5 (23%)

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	GLC	A	998	-	-	2/2/22/22	0/1/1/1
3	AMP	A	997	-	-	0/10/26/26	0/3/3/3
4	PLP	A	999	1	-	3/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	PLP	C4A-C4	-6.76	1.38	1.51
4	A	999	PLP	C5-C4	-4.07	1.35	1.40
4	A	999	PLP	C3-C2	-2.95	1.37	1.41
4	A	999	PLP	C2A-C2	2.45	1.54	1.50
4	A	999	PLP	C2-N1	2.06	1.37	1.33
4	A	999	PLP	C3-C4	-2.04	1.36	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	PLP	O4P-C5A-C5	2.86	114.72	109.36
4	A	999	PLP	O2P-P-O4P	-2.83	99.29	106.67
4	A	999	PLP	C6-C5-C4	2.30	119.98	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	PLP	O3P-P-O2P	2.27	116.33	107.80
4	A	999	PLP	C5-C6-N1	-2.21	120.24	123.83
3	A	997	AMP	O2P-P-O5'	-2.12	101.13	106.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

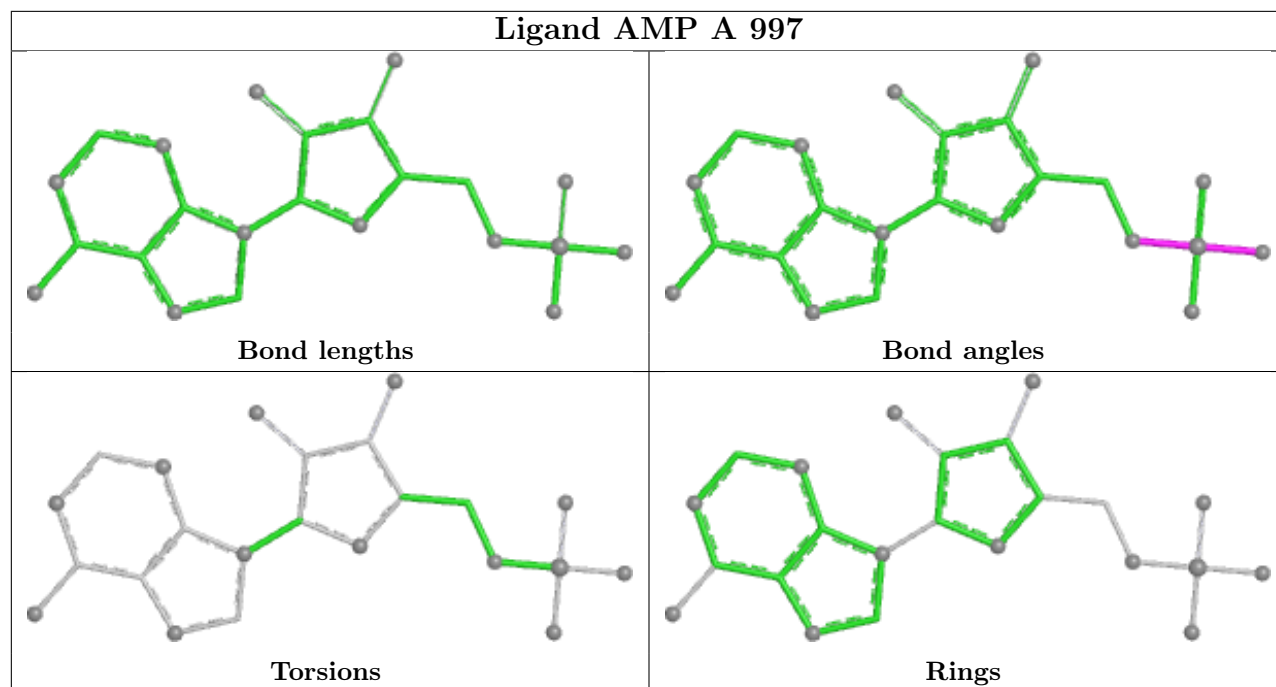
Mol	Chain	Res	Type	Atoms
4	A	999	PLP	C5A-O4P-P-O2P
4	A	999	PLP	C5A-O4P-P-O3P
2	A	998	GLC	O5-C5-C6-O6
2	A	998	GLC	C4-C5-C6-O6
4	A	999	PLP	C5A-O4P-P-O1P

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	998	GLC	5	0
3	A	997	AMP	1	0
4	A	999	PLP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	318:SER	C	319:THR	N	1.72
1	A	320:ARG	C	321:GLY	N	1.19
1	A	319:THR	C	320:ARG	N	1.16
1	A	321:GLY	C	322:ALA	N	0.75

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	833/846 (98%)	0.49	69 (8%) 17 14	24, 51, 90, 110	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	THR	6.4
1	A	267	LEU	4.7
1	A	379	VAL	4.6
1	A	21	VAL	4.5
1	A	5	THR	4.4
1	A	378	THR	4.3
1	A	380	LEU	4.2
1	A	593	ASP	4.2
1	A	728	ALA	4.1
1	A	597	LEU	4.1
1	A	383	ALA	3.9
1	A	321	GLY	3.9
1	A	838	ASN	3.8
1	A	316	PHE	3.5
1	A	837	SER	3.4
1	A	436	SER	3.4
1	A	322	ALA	3.1
1	A	6	ASP	3.1
1	A	594	PRO	3.1
1	A	777	TYR	2.9
1	A	669	ALA	2.9
1	A	384	LEU	2.9
1	A	766	PHE	2.9
1	A	318	SER	2.7
1	A	320	ARG	2.7
1	A	476	PRO	2.7
1	A	715	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	581	LEU	2.7
1	A	596	LYS	2.6
1	A	732	TYR	2.6
1	A	578	LEU	2.6
1	A	174	TRP	2.6
1	A	8	GLU	2.5
1	A	764	MET	2.5
1	A	599	VAL	2.5
1	A	418	PHE	2.4
1	A	711	PHE	2.4
1	A	753	LYS	2.3
1	A	248	ALA	2.3
1	A	733	GLU	2.3
1	A	761	ILE	2.3
1	A	832	LEU	2.3
1	A	257	PHE	2.3
1	A	325	VAL	2.3
1	A	555	VAL	2.3
1	A	255	ARG	2.3
1	A	736	PRO	2.3
1	A	271	LEU	2.2
1	A	414	ILE	2.2
1	A	595	LYS	2.2
1	A	173	GLY	2.2
1	A	323	GLY	2.2
1	A	264	GLN	2.2
1	A	431	ILE	2.2
1	A	181	ASP	2.2
1	A	769	ASP	2.2
1	A	381	PRO	2.1
1	A	592	LYS	2.1
1	A	792	MET	2.1
1	A	251	ASP	2.1
1	A	286	PHE	2.1
1	A	532	ARG	2.1
1	A	724	LYS	2.1
1	A	755	PRO	2.1
1	A	725	GLY	2.0
1	A	422	VAL	2.0
1	A	435	GLY	2.0
1	A	742	ILE	2.0
1	A	767	TYR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	14	10/11	0.98	0.05	30,35,38,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

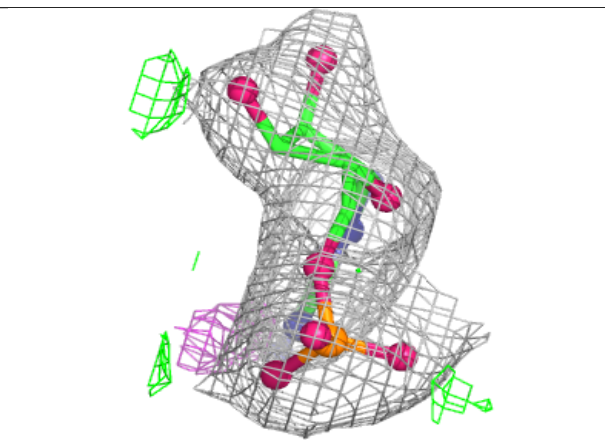
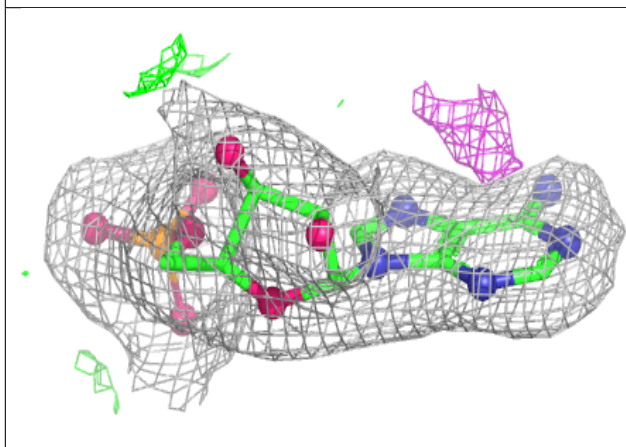
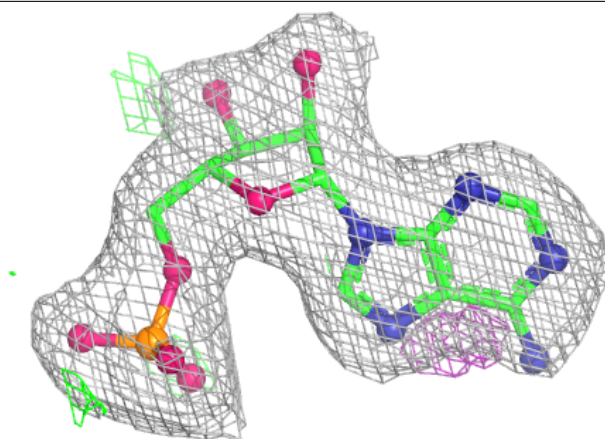
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	A	998	12/12	0.84	0.17	62,82,98,98	0
3	AMP	A	997	23/23	0.95	0.07	30,40,48,54	0
4	PLP	A	999	15/16	0.95	0.07	26,36,58,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AMP A 997:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.