



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:55 AM UTC

PDB ID : 1A8I / pdb_00001a8i
Title : SPIROHYDANTOIN INHIBITOR OF GLYCOGEN PHOSPHORYLASE
Authors : Gregoriou, M.; Noble, M.E.M.; Watson, K.A.; Garman, E.F.; Krulle, T.M.;
De La Fuente, C.; Fleet, G.W.J.; Oikonomakos, N.G.; Johnson, L.N.
Deposited on : 1998-03-25
Resolution : 1.78 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
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

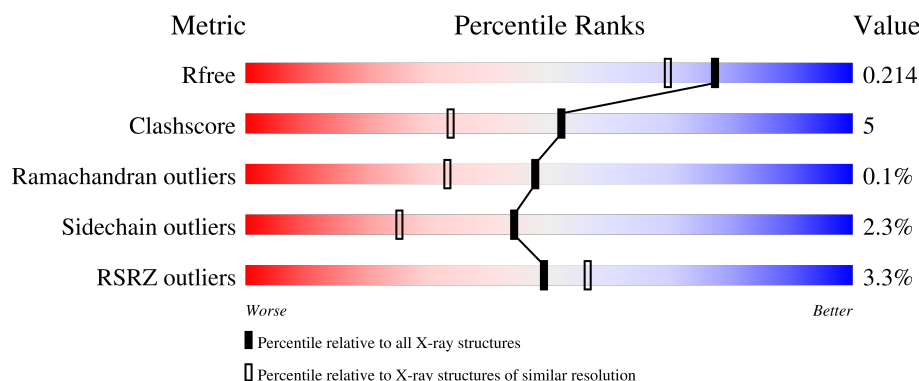
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	842	 3% 77% 17% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7454 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.

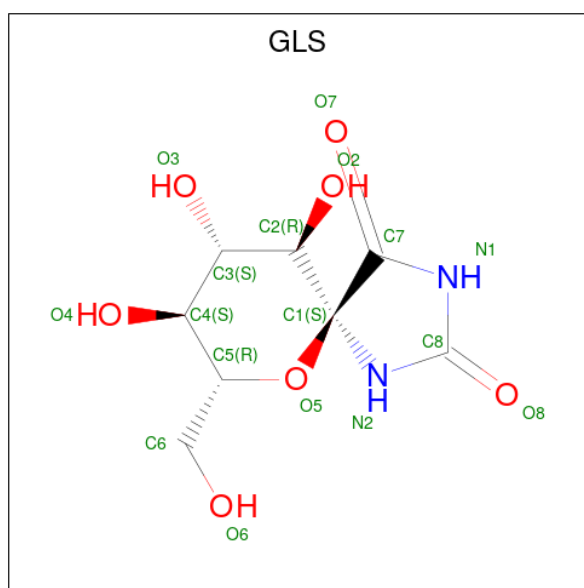
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	813	6642	4232	1173	1207	1	29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	SEE REMARK 999	UNP P00489
A	680	LLP	LYS	modified residue	UNP P00489

- Molecule 2 is BETA-D-GLUCOPYRANOSE SPIROHYDANTOIN (CCD ID: GLS) (formula: $C_8H_{12}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	17	8	2	7	0	0

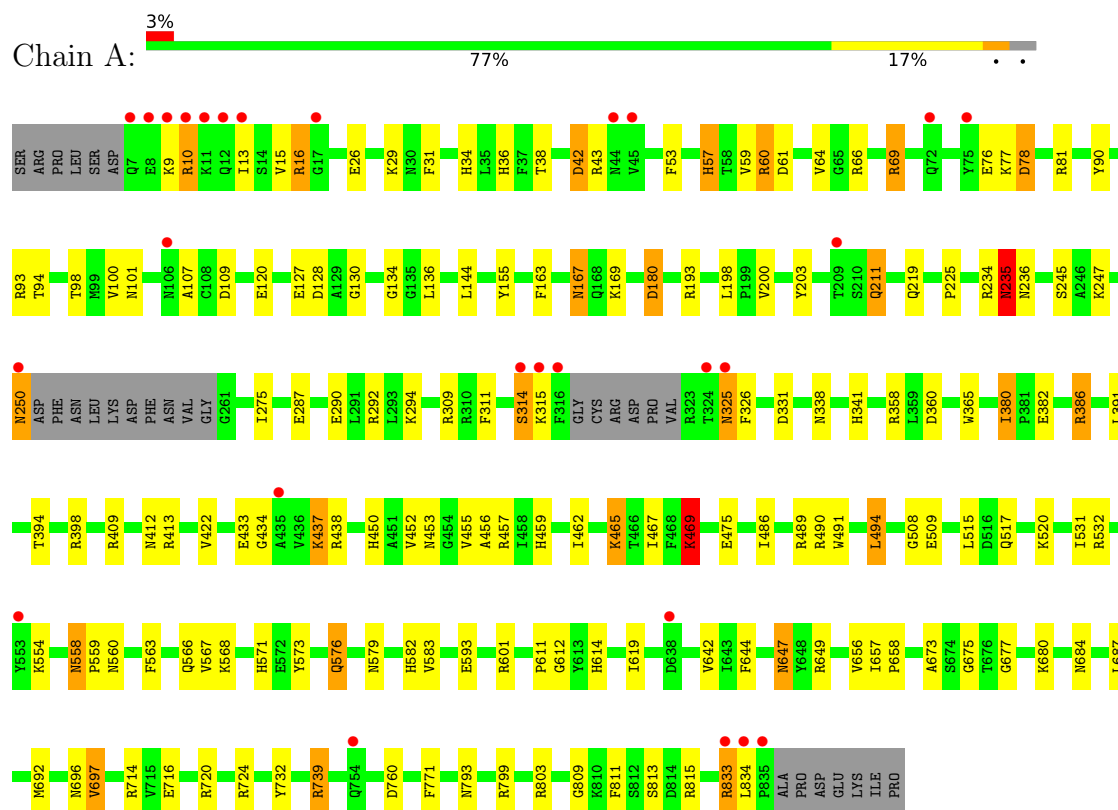
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	795	Total 795	O 795	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 B



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.47Å 127.47Å 115.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.78 19.90 – 1.78	Depositor EDS
% Data completeness (in resolution range)	86.4 (19.90-1.78) 86.4 (19.90-1.78)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.78Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.229 0.170 , 0.214	Depositor DCC
R_{free} test set	3967 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7454	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: LLP, GLS

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	1.06	3/6764 (0.0%)	1.82	136/9147 (1.5%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	GLY	N-CA	6.04	1.54	1.44
1	A	815	ARG	NE-CZ	5.91	1.39	1.33
1	A	813	SER	C-N	5.21	1.40	1.33

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ARG	CD-NE-CZ	22.56	155.99	124.40
1	A	81	ARG	CD-NE-CZ	18.94	150.91	124.40
1	A	380	ILE	N-CA-CB	-12.84	96.76	109.99
1	A	42	ASP	CA-CB-CG	12.17	124.77	112.60
1	A	386	ARG	NE-CZ-NH2	11.07	129.16	119.20
1	A	532	ARG	CD-NE-CZ	10.33	138.86	124.40
1	A	234	ARG	CD-NE-CZ	9.90	138.26	124.40
1	A	155	TYR	CA-C-O	-9.66	109.89	120.33
1	A	811	PHE	CA-CB-CG	-8.97	104.83	113.80
1	A	611	PRO	CA-C-N	-8.65	109.83	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	PRO	C-N-CA	-8.65	109.83	122.46
1	A	833	ARG	CD-NE-CZ	8.23	135.93	124.40
1	A	167	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	A	386	ARG	NE-CZ-NH1	-7.99	113.51	121.50
1	A	649	ARG	NE-CZ-NH1	7.95	129.45	121.50
1	A	687	LEU	O-C-N	7.93	131.99	123.03
1	A	235	ASN	OD1-CG-ND2	7.73	130.33	122.60
1	A	438	ARG	CD-NE-CZ	7.65	135.11	124.40
1	A	815	ARG	NE-CZ-NH2	-7.54	112.42	119.20
1	A	453	ASN	O-C-N	7.37	131.81	123.27
1	A	457	ARG	NE-CZ-NH2	-7.37	112.57	119.20
1	A	31	PHE	CA-CB-CG	7.35	121.15	113.80
1	A	43	ARG	NE-CZ-NH2	7.21	125.69	119.20
1	A	98	THR	O-C-N	7.09	129.75	122.09
1	A	714	ARG	NE-CZ-NH2	-7.09	112.82	119.20
1	A	250	ASN	CA-C-O	7.07	132.82	120.80
1	A	687	LEU	CA-C-N	-7.02	112.75	122.93
1	A	687	LEU	C-N-CA	-7.02	112.75	122.93
1	A	163	PHE	CA-CB-CG	-6.95	106.85	113.80
1	A	53	PHE	CA-CB-CG	-6.92	106.88	113.80
1	A	69	ARG	CD-NE-CZ	6.88	134.04	124.40
1	A	101	ASN	CA-CB-CG	-6.84	105.76	112.60
1	A	469	LYS	CA-C-O	-6.79	113.30	120.63
1	A	579	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	793	ASN	CA-CB-CG	6.70	119.30	112.60
1	A	452	VAL	O-C-N	-6.63	116.04	123.20
1	A	457	ARG	NH1-CZ-NH2	6.62	127.91	119.30
1	A	687	LEU	CA-C-O	-6.56	113.66	121.66
1	A	200	VAL	O-C-N	6.55	130.11	123.10
1	A	475	GLU	CA-C-N	6.51	126.44	119.28
1	A	475	GLU	C-N-CA	6.51	126.44	119.28
1	A	614	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	294	LYS	O-C-N	6.43	128.93	122.12
1	A	250	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	78	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	489	ARG	NE-CZ-NH1	6.31	127.81	121.50
1	A	716	GLU	CB-CG-CD	6.30	123.31	112.60
1	A	486	ILE	CA-C-O	-6.25	114.65	121.28
1	A	127	GLU	CA-C-O	-6.24	113.74	120.92
1	A	325	ASN	CA-C-O	-6.23	111.60	120.51
1	A	128	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	739	ARG	NE-CZ-NH2	6.18	124.76	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	573	TYR	O-C-N	6.17	130.69	122.43
1	A	93	ARG	NH1-CZ-NH2	6.12	127.25	119.30
1	A	566	GLN	OE1-CD-NE2	6.09	128.69	122.60
1	A	697	VAL	CB-CA-C	-6.06	104.21	111.97
1	A	647	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	A	799	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	A	98	THR	CA-C-O	-6.02	114.50	120.70
1	A	294	LYS	CA-C-O	-5.97	114.22	120.55
1	A	673	ALA	O-C-N	5.95	128.42	122.12
1	A	601	ARG	CA-C-O	5.92	127.93	121.06
1	A	380	ILE	CB-CA-C	5.90	116.78	111.00
1	A	331	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	341	HIS	O-C-N	-5.88	114.87	120.70
1	A	155	TYR	CA-C-N	-5.82	115.93	121.57
1	A	155	TYR	C-N-CA	-5.82	115.93	121.57
1	A	422	VAL	CA-C-O	-5.80	114.71	120.85
1	A	64	VAL	N-CA-C	5.78	115.97	110.42
1	A	453	ASN	CA-C-O	-5.76	114.37	121.06
1	A	326	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	365	TRP	CA-C-O	5.75	126.51	120.42
1	A	515	LEU	N-CA-C	5.74	119.39	112.38
1	A	134	GLY	CA-C-N	5.72	126.29	119.94
1	A	134	GLY	C-N-CA	5.72	126.29	119.94
1	A	292	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	A	456	ALA	N-CA-CB	5.71	120.32	111.24
1	A	724	ARG	CD-NE-CZ	-5.71	116.41	124.40
1	A	582	HIS	CA-C-O	5.69	126.80	120.82
1	A	809	GLY	N-CA-C	5.64	119.71	112.83
1	A	315	LYS	CA-CB-CG	5.62	125.34	114.10
1	A	326	PHE	N-CA-C	5.62	118.17	111.71
1	A	287	GLU	O-C-N	-5.59	116.08	123.13
1	A	57	HIS	O-C-N	5.57	128.50	122.15
1	A	696	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	677	GLY	N-CA-C	-5.54	106.08	112.73
1	A	649	ARG	CA-C-O	-5.54	115.35	121.28
1	A	309	ARG	CD-NE-CZ	5.52	132.13	124.40
1	A	803	ARG	O-C-N	5.52	128.68	122.22
1	A	508	GLY	O-C-N	5.52	128.15	122.91
1	A	107	ALA	CA-C-O	5.48	126.35	120.70
1	A	558	ASN	CA-C-O	5.48	123.68	119.46
1	A	560	ASN	CA-CB-CG	-5.48	107.12	112.60
1	A	563	PHE	CA-CB-CG	5.46	119.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ASP	CB-CA-C	5.45	121.56	109.94
1	A	236	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	593	GLU	CA-C-N	5.45	125.27	119.28
1	A	593	GLU	C-N-CA	5.45	125.27	119.28
1	A	644	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	26	GLU	CB-CG-CD	5.41	121.80	112.60
1	A	517	GLN	O-C-N	-5.40	115.25	122.43
1	A	211	GLN	N-CA-C	-5.37	105.95	112.88
1	A	398	ARG	CD-NE-CZ	5.34	131.88	124.40
1	A	180	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	341	HIS	CA-C-N	5.30	126.47	119.84
1	A	341	HIS	C-N-CA	5.30	126.47	119.84
1	A	489	ARG	NH1-CZ-NH2	-5.30	112.42	119.30
1	A	225	PRO	CA-C-N	5.29	130.47	123.00
1	A	225	PRO	C-N-CA	5.29	130.47	123.00
1	A	93	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	A	36	HIS	CA-CB-CG	5.28	119.08	113.80
1	A	338	ASN	O-C-N	5.27	129.38	122.68
1	A	198	LEU	O-C-N	5.27	125.66	121.55
1	A	394	THR	O-C-N	5.25	127.76	122.09
1	A	275	ILE	CA-C-O	-5.22	115.52	120.95
1	A	803	ARG	CA-C-O	-5.21	114.21	120.10
1	A	675	GLY	CA-C-O	-5.20	117.72	122.24
1	A	412	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	94	THR	CA-CB-CG2	5.18	119.31	110.50
1	A	234	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	A	467	ILE	N-CA-C	5.16	115.78	110.36
1	A	567	VAL	N-CA-CB	5.16	118.84	111.82
1	A	438	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	360	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	771	PHE	N-CA-C	5.09	119.19	112.92
1	A	59	VAL	CA-C-O	5.09	126.25	120.85
1	A	684	ASN	CA-CB-CG	-5.08	107.52	112.60
1	A	60	ARG	N-CA-C	5.07	116.81	111.28
1	A	16	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	A	203	TYR	CB-CA-C	-5.04	110.78	116.63
1	A	193	ARG	CA-C-N	5.04	124.82	119.28
1	A	193	ARG	C-N-CA	5.04	124.82	119.28
1	A	834	LEU	N-CA-C	-5.02	103.36	110.29
1	A	531	ILE	CA-C-O	5.01	126.48	121.27
1	A	656	VAL	N-CA-C	5.00	118.15	111.44
1	A	614	HIS	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	491	TRP	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	6642	0	6593	67	0
2	A	17	0	12	0	0
3	A	795	0	0	20	3
All	All	7454	0	6605	67	3

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 5.

All (67) 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:490:ARG:HA	1:A:494:LEU:HG	1.50	0.92
1:A:100:VAL:HG21	1:A:494:LEU:HD22	1.64	0.79
1:A:60:ARG:HD2	3:A:1103:HOH:O	1.82	0.78
1:A:211:GLN:HB3	1:A:358:ARG:HH22	1.49	0.77
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.75	0.69
1:A:455:VAL:H	1:A:459:HIS:HD2	1.44	0.65
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.79	0.65
1:A:9:LYS:HG3	1:A:13:ILE:HD11	1.78	0.64
1:A:450:HIS:HD2	3:A:1339:HOH:O	1.80	0.63
1:A:692:MET:HE1	1:A:697:VAL:HG13	1.79	0.62
1:A:386:ARG:NH1	3:A:1439:HOH:O	2.32	0.61
1:A:211:GLN:HB3	1:A:358:ARG:NH2	2.15	0.61
1:A:60:ARG:HD3	3:A:1428:HOH:O	2.00	0.60
1:A:311:PHE:CE2	1:A:325:ASN:HB2	2.36	0.60
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.85	0.60
1:A:100:VAL:HG21	1:A:494:LEU:CD2	2.33	0.58
1:A:583:VAL:HG11	1:A:642:VAL:HG21	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:H	1:A:235:ASN:HD22	1.52	0.56
1:A:450:HIS:HE1	3:A:1328:HOH:O	1.90	0.55
1:A:211:GLN:HE21	1:A:358:ARG:NH2	2.05	0.54
1:A:433:GLU:HG3	1:A:434:GLY:H	1.75	0.52
1:A:311:PHE:HE2	1:A:325:ASN:HB2	1.74	0.52
1:A:211:GLN:CB	1:A:358:ARG:HH22	2.22	0.51
1:A:380:ILE:CG2	1:A:382:GLU:CD	2.84	0.51
1:A:380:ILE:HG23	1:A:382:GLU:OE1	2.12	0.50
1:A:69:ARG:NH2	3:A:1182:HOH:O	2.44	0.50
1:A:386:ARG:NH2	3:A:1090:HOH:O	2.45	0.50
1:A:78:ASP:OD1	1:A:314:SER:HB2	2.12	0.49
1:A:619:ILE:HD13	3:A:1196:HOH:O	2.13	0.48
1:A:16:ARG:HD3	3:A:1694:HOH:O	2.13	0.48
1:A:583:VAL:CG1	1:A:642:VAL:HG21	2.44	0.48
1:A:10:ARG:HB3	3:A:1694:HOH:O	2.14	0.48
1:A:554:LYS:HG3	3:A:1130:HOH:O	2.14	0.48
1:A:167:ASN:HD22	1:A:647:ASN:HD21	1.61	0.47
1:A:10:ARG:HE	1:A:109:ASP:CG	2.23	0.47
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.49	0.46
1:A:10:ARG:NH1	3:A:1050:HOH:O	2.39	0.46
1:A:167:ASN:ND2	1:A:647:ASN:HD21	2.13	0.46
1:A:760:ASP:HB2	3:A:1735:HOH:O	2.16	0.46
1:A:15:VAL:HA	1:A:509:GLU:OE2	2.16	0.45
1:A:520:LYS:NZ	3:A:1564:HOH:O	2.47	0.45
1:A:692:MET:HE3	1:A:697:VAL:HG22	1.99	0.45
1:A:10:ARG:NH1	1:A:120:GLU:HG3	2.31	0.44
1:A:57:HIS:HE1	3:A:1506:HOH:O	2.00	0.44
1:A:380:ILE:HG23	1:A:382:GLU:CD	2.41	0.44
1:A:437:LYS:HE2	1:A:437:LYS:HB3	1.83	0.44
1:A:10:ARG:NH2	1:A:109:ASP:OD1	2.44	0.43
1:A:469:LYS:HZ2	1:A:469:LYS:HB3	1.82	0.43
1:A:219:GLN:HG2	3:A:1106:HOH:O	2.17	0.43
1:A:409:ARG:HH11	1:A:409:ARG:HD3	1.63	0.43
1:A:433:GLU:HG3	1:A:434:GLY:N	2.34	0.43
1:A:462:ILE:HD12	1:A:462:ILE:HA	1.93	0.42
1:A:833:ARG:NH2	3:A:1737:HOH:O	2.52	0.42
1:A:136:LEU:C	1:A:136:LEU:HD23	2.43	0.42
1:A:692:MET:CE	1:A:697:VAL:HG13	2.48	0.42
1:A:211:GLN:CG	1:A:358:ARG:HH22	2.33	0.42
1:A:100:VAL:CG2	1:A:494:LEU:HD22	2.42	0.41
1:A:657:ILE:N	1:A:658:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:HIS:H	1:A:576:GLN:HE22	1.68	0.41
1:A:90:TYR:CE1	1:A:130:GLY:HA2	2.56	0.41
1:A:720:ARG:NH1	3:A:1174:HOH:O	2.53	0.41
1:A:465:LYS:HZ2	1:A:465:LYS:HG2	1.69	0.41
1:A:245:SER:OG	1:A:247:LYS:NZ	2.54	0.40
1:A:413:ARG:HD3	3:A:1342:HOH:O	2.21	0.40
1:A:558:ASN:HA	1:A:559:PRO:HD2	1.93	0.40
1:A:10:ARG:HD3	3:A:1050:HOH:O	2.21	0.40
1:A:66:ARG:HH11	1:A:66:ARG:HD2	1.64	0.40

All (3) 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)
3:A:1173:HOH:O	3:A:1173:HOH:O[7_556]	1.83	0.37
3:A:1065:HOH:O	3:A:1521:HOH:O[7_556]	1.94	0.26
3:A:1254:HOH:O	3:A:1648:HOH:O[7_555]	2.04	0.16

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	806/842 (96%)	777 (96%)	28 (4%)	1 (0%)	48 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	SER

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	704/730 (96%)	688 (98%)	16 (2%)	44 25

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	29	LYS
1	A	42	ASP
1	A	76	GLU
1	A	77	LYS
1	A	144	LEU
1	A	169	LYS
1	A	180	ASP
1	A	235	ASN
1	A	250	ASN
1	A	437	LYS
1	A	465	LYS
1	A	469	LYS
1	A	494	LEU
1	A	568	LYS
1	A	576	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	57	HIS
1	A	96	GLN
1	A	106	ASN
1	A	167	ASN
1	A	211	GLN
1	A	235	ASN
1	A	284	ASN
1	A	450	HIS

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Mol	Chain	Res	Type
1	A	459	HIS
1	A	496	ASN
1	A	541	ASN
1	A	560	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	767	HIS

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	LLP	A	680	1	23,24,25	2.65	6 (26%)	25,32,34	1.95	7 (28%)

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	LLP	A	680	1	-	2/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	C3-C2	-6.58	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	C4'-NZ	6.46	1.48	1.27
1	A	680	LLP	C2-N1	5.14	1.43	1.33
1	A	680	LLP	P-OP3	-3.57	1.41	1.54
1	A	680	LLP	C4-C3	-2.92	1.36	1.41
1	A	680	LLP	C4-C4'	2.46	1.51	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	C4-C3-C2	4.91	122.91	120.14
1	A	680	LLP	C2'-C2-C3	3.47	124.86	120.80
1	A	680	LLP	OP4-C5'-C5	-2.80	104.11	109.36
1	A	680	LLP	C6-N1-C2	-2.71	114.28	119.20
1	A	680	LLP	CG-CD-CE	-2.60	104.34	113.38
1	A	680	LLP	C5-C4-C4'	-2.52	117.58	121.47
1	A	680	LLP	C5'-C5-C6	2.35	123.19	119.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	680	LLP	C4-C5-C5'-OP4
1	A	680	LLP	C6-C5-C5'-OP4

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 [i](#)

1 ligand 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	$\# Z > 2$
2	GLS	A	998	-	15,18,18	0.94	1 (6%)	19,28,28	3.11	7 (36%)

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	GLS	A	998	-	-	0/2/40/40	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	GLS	C8-N1	-2.25	1.33	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	GLS	N1-C8-N2	8.17	116.52	107.56
2	A	998	GLS	C7-N1-C8	-7.36	104.18	111.69
2	A	998	GLS	O7-C7-N1	-3.77	121.07	126.17
2	A	998	GLS	C4-C3-C2	-2.99	106.91	111.18
2	A	998	GLS	O3-C3-C2	-2.96	103.59	109.77
2	A	998	GLS	O8-C8-N2	-2.68	122.50	126.60
2	A	998	GLS	O8-C8-N1	-2.52	120.98	125.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	812/842 (96%)	-0.03	27 (3%) 49 56	15, 23, 45, 100	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	GLN	6.5
1	A	324	THR	6.3
1	A	834	LEU	5.8
1	A	835	PRO	4.7
1	A	435	ALA	4.6
1	A	10	ARG	4.6
1	A	316	PHE	4.1
1	A	13	ILE	3.8
1	A	12	GLN	3.8
1	A	8	GLU	3.6
1	A	325	ASN	3.6
1	A	17	GLY	3.5
1	A	9	LYS	3.4
1	A	44	ASN	3.3
1	A	11	LYS	3.1
1	A	314	SER	2.9
1	A	833	ARG	2.7
1	A	45	VAL	2.5
1	A	315	LYS	2.5
1	A	553	TYR	2.5
1	A	75	TYR	2.4
1	A	209	THR	2.3
1	A	72	GLN	2.3
1	A	638	ASP	2.2
1	A	754	GLN	2.2
1	A	250	ASN	2.2
1	A	106	ASN	2.1

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	LLP	A	680	24/25	0.97	0.05	14,17,19,20	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	GLS	A	998	17/17	0.98	0.04	12,15,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.