



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:50 AM UTC

PDB ID : 6GPB / pdb_00006gpb
Title : REFINED CRYSTAL STRUCTURE OF THE PHOSPHORYLASE-HEPTULOSE 2-PHOSPHATE-OLIGOSACCHARIDE-AMP COMPLEX
Authors : Acharya, K.R.; Johnson, L.N.
Deposited on : 1990-06-04
Resolution : 2.86 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

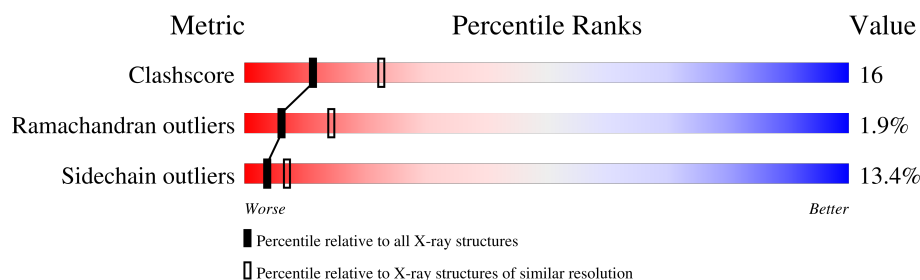
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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))
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	
2	B	5	

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
3	H2P	A	998	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7469 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.

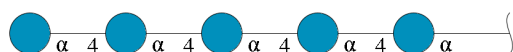
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	828	Total	C	N	O	S	0	0	0
			6727	4286	1186	1225	30			

There is a discrepancy between the modelled and reference sequences:

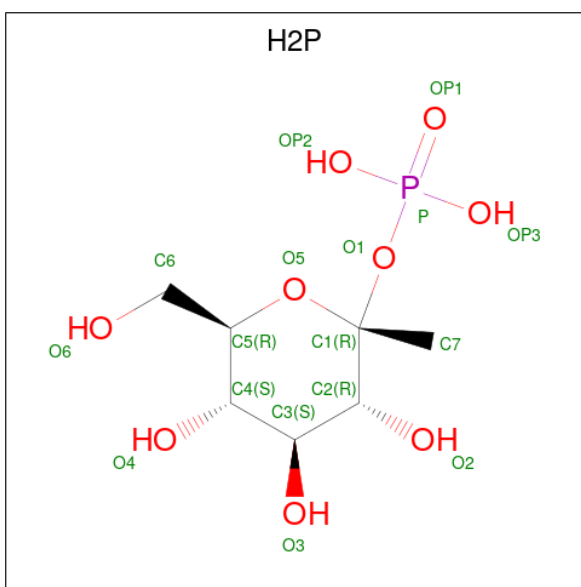
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



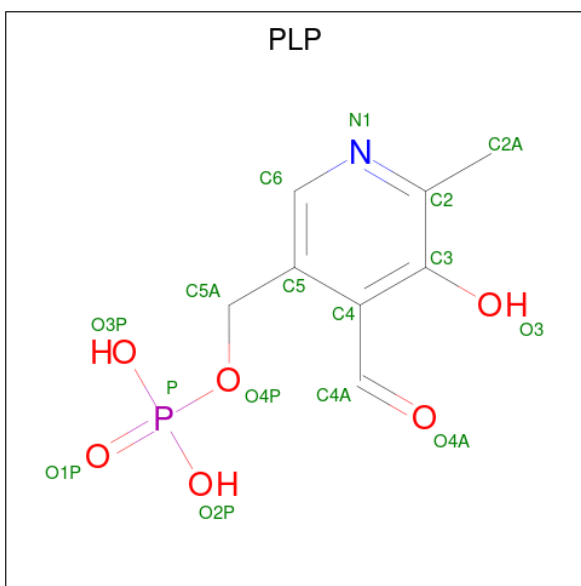
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is 1-deoxy-2-O-phosphono-alpha-D-glucopyranose (CCD ID: H2P) (formula: C₇H₁₅O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			17	7	9	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 ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 6 is water.

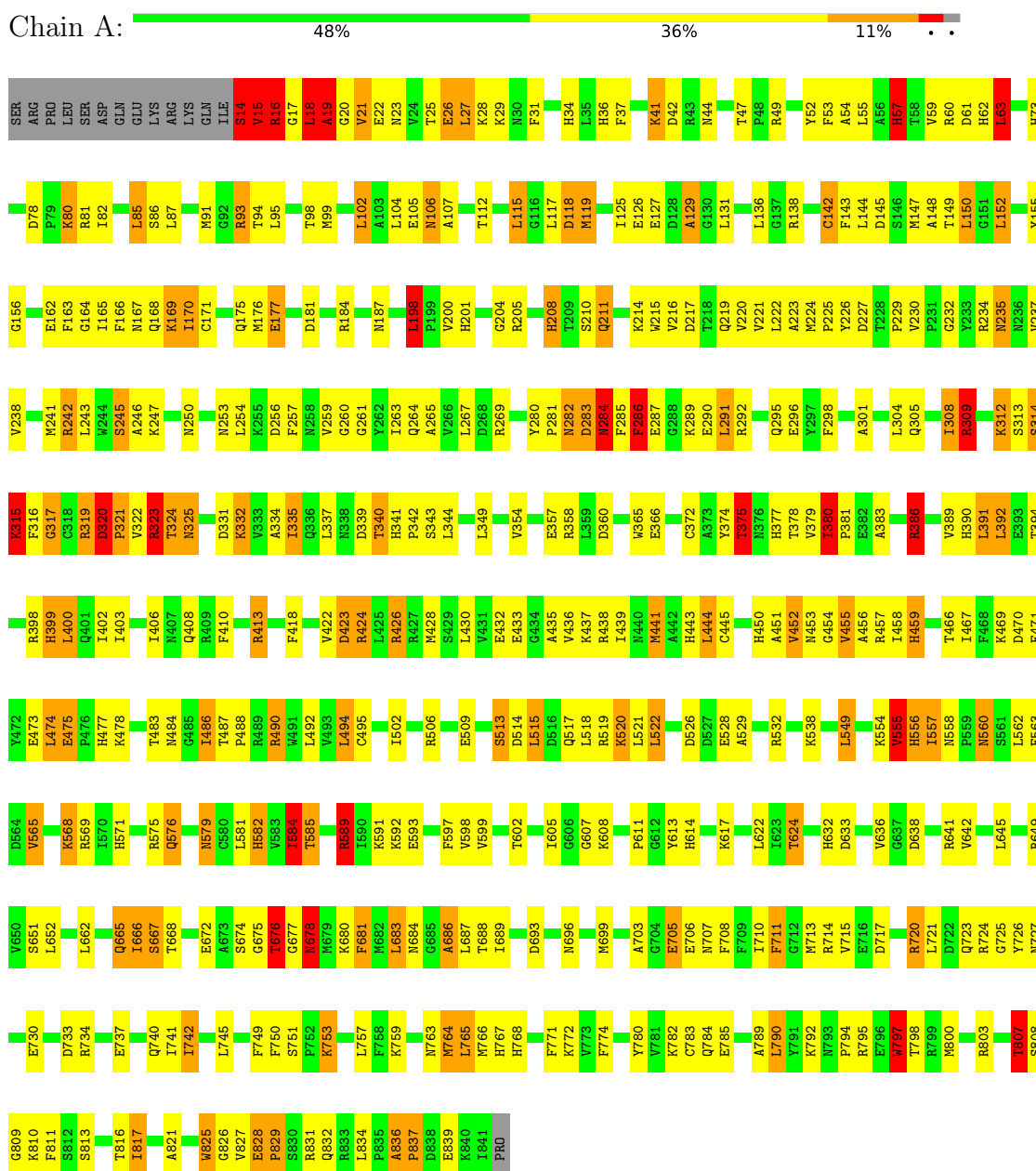
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	608	Total	O	0	0
			608	608		

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. 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. 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.

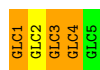
Note EDS was not executed.

• Molecule 1: GLYCOGEN PHOSPHORYLASE B



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain B:  20% 20% 60%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.50Å 128.50Å 116.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.86	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.86)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7469	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, H2P, GLC, 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	1.91	67/6880 (1.0%)	2.14	308/9313 (3.3%)

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	9

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	ARG	C-O	80.71	2.16	1.24
1	A	18	LEU	CG-CD1	42.68	2.93	1.52
1	A	18	LEU	CA-C	39.85	2.00	1.52
1	A	282	ASN	C-N	-31.16	0.94	1.33
1	A	312	LYS	CE-NZ	28.61	2.35	1.49
1	A	15	VAL	CA-C	26.70	1.86	1.52
1	A	19	ALA	N-CA	-21.90	1.18	1.46
1	A	286	PHE	C-N	20.26	1.59	1.33
1	A	18	LEU	CB-CG	-18.16	1.17	1.53
1	A	41	LYS	C-N	-14.88	1.13	1.33
1	A	317	GLY	CA-C	-14.62	1.27	1.51
1	A	15	VAL	N-CA	-12.19	1.31	1.46
1	A	14	SER	CA-CB	11.66	1.76	1.53
1	A	281	PRO	C-N	-11.62	1.17	1.33
1	A	17	GLY	N-CA	-10.98	1.26	1.45
1	A	14	SER	C-N	10.49	1.48	1.33
1	A	57	HIS	CE1-NE2	-10.47	1.22	1.32
1	A	284	ASN	N-CA	10.19	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	LEU	CG-CD2	9.58	1.84	1.52
1	A	14	SER	CA-C	-8.88	1.34	1.52
1	A	332	LYS	CE-NZ	8.42	1.74	1.49
1	A	18	LEU	N-CA	8.39	1.56	1.45
1	A	15	VAL	CA-CB	8.29	1.65	1.54
1	A	319	ARG	CB-CG	-7.62	1.29	1.52
1	A	57	HIS	CD2-NE2	-7.30	1.29	1.37
1	A	19	ALA	CA-CB	-7.28	1.41	1.53
1	A	16	ARG	CZ-NH2	7.23	1.42	1.33
1	A	614	HIS	CD2-NE2	-6.98	1.30	1.37
1	A	443	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	57	HIS	CG-ND1	-6.61	1.30	1.38
1	A	14	SER	N-CA	6.60	1.58	1.46
1	A	19	ALA	CA-C	-6.59	1.44	1.52
1	A	477	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	632	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	767	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	582	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	556	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	399	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	459	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	62	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	768	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	450	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	208	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	571	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	36	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	390	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	20	GLY	CA-C	5.81	1.60	1.51
1	A	16	ARG	NE-CZ	5.72	1.39	1.33
1	A	377	HIS	CD2-NE2	-5.71	1.31	1.37
1	A	87	LEU	C-N	-5.69	1.24	1.33
1	A	201	HIS	CD2-NE2	-5.68	1.31	1.37
1	A	315	LYS	N-CA	-5.66	1.38	1.46
1	A	14	SER	C-O	5.64	1.34	1.23
1	A	57	HIS	ND1-CE1	-5.63	1.26	1.32
1	A	319	ARG	CA-CB	-5.58	1.46	1.53
1	A	34	HIS	CD2-NE2	-5.53	1.31	1.37
1	A	341	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	308	ILE	C-N	-5.48	1.27	1.33
1	A	208	HIS	CG-ND1	-5.42	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	ASP	CA-C	5.41	1.59	1.53
1	A	319	ARG	CZ-NH1	-5.36	1.25	1.32
1	A	459	HIS	CG-ND1	-5.26	1.32	1.38
1	A	16	ARG	CB-CG	-5.22	1.36	1.52
1	A	443	HIS	CG-ND1	-5.22	1.32	1.38
1	A	377	HIS	CG-ND1	-5.10	1.32	1.38
1	A	57	HIS	CB-CG	-5.06	1.43	1.50

All (308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LEU	CA-C-N	21.88	163.32	121.54
1	A	18	LEU	C-N-CA	21.88	163.32	121.54
1	A	257	PHE	N-CA-C	-18.46	88.29	110.44
1	A	16	ARG	CA-CB-CG	17.93	149.96	114.10
1	A	286	PHE	O-C-N	-16.28	104.82	123.06
1	A	284	ASN	CA-C-O	16.15	143.61	120.51
1	A	678	ASN	CA-CB-CG	14.82	127.42	112.60
1	A	19	ALA	CA-C-N	13.60	148.06	121.41
1	A	19	ALA	C-N-CA	13.60	148.06	121.41
1	A	322	VAL	N-CA-C	-13.08	100.31	111.56
1	A	323	ARG	N-CA-C	-13.06	82.98	110.80
1	A	14	SER	N-CA-CB	12.52	131.78	110.50
1	A	19	ALA	N-CA-CB	12.45	131.53	110.49
1	A	281	PRO	O-C-N	-11.77	106.75	122.64
1	A	14	SER	O-C-N	-11.66	104.34	123.00
1	A	683	LEU	N-CA-C	-11.52	92.50	110.36
1	A	259	VAL	N-CA-C	-11.05	92.07	109.20
1	A	834	LEU	N-CA-C	-11.05	96.02	110.39
1	A	807	THR	N-CA-CB	-10.81	94.48	110.49
1	A	386	ARG	N-CA-C	-10.54	91.05	108.34
1	A	31	PHE	N-CA-C	-10.40	99.91	111.14
1	A	20	GLY	CA-C-O	-9.91	103.32	120.57
1	A	254	LEU	N-CA-C	-9.66	99.38	112.03
1	A	57	HIS	CA-CB-CG	-9.65	104.15	113.80
1	A	652	LEU	N-CA-C	-9.62	100.30	112.90
1	A	215	TRP	N-CA-C	-9.42	93.83	109.46
1	A	107	ALA	N-CA-C	-9.40	99.93	111.40
1	A	18	LEU	CD1-CG-CD2	-9.34	90.25	110.80
1	A	554	LYS	N-CA-C	-9.33	93.43	108.55
1	A	324	THR	N-CA-C	-9.25	91.09	110.80
1	A	221	VAL	N-CA-C	-9.18	94.71	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLY	N-CA-C	9.11	128.97	112.02
1	A	668	THR	N-CA-C	-9.06	96.36	109.96
1	A	676	THR	N-CA-CB	-8.85	99.14	110.90
1	A	711	PHE	N-CA-C	-8.84	96.76	108.34
1	A	562	LEU	N-CA-C	-8.80	95.77	109.76
1	A	423	ASP	CA-CB-CG	-8.59	104.01	112.60
1	A	16	ARG	N-CA-C	-8.56	102.15	112.59
1	A	15	VAL	O-C-N	8.54	133.24	122.57
1	A	15	VAL	CA-C-O	8.51	131.42	120.78
1	A	317	GLY	O-C-N	8.27	134.34	122.68
1	A	571	HIS	CB-CG-CD2	-8.17	120.58	131.20
1	A	176	MET	N-CA-C	-8.14	95.63	108.90
1	A	324	THR	O-C-N	-8.09	111.83	122.59
1	A	14	SER	CA-CB-OG	8.02	127.14	111.10
1	A	831	ARG	N-CA-C	-7.97	103.12	112.92
1	A	19	ALA	N-CA-C	7.96	127.76	110.80
1	A	16	ARG	NE-CZ-NH2	7.94	126.35	119.20
1	A	15	VAL	CB-CA-C	-7.93	98.28	111.29
1	A	47	THR	N-CA-C	-7.86	100.88	110.31
1	A	452	VAL	N-CA-C	-7.86	96.70	108.17
1	A	589	ARG	N-CA-C	-7.82	102.71	111.07
1	A	219	GLN	N-CA-C	-7.81	97.60	110.17
1	A	314	SER	O-C-N	7.81	132.62	123.02
1	A	651	SER	CA-CB-OG	-7.80	95.49	111.10
1	A	18	LEU	CA-CB-CG	-7.79	89.05	116.30
1	A	331	ASP	N-CA-C	-7.77	103.81	113.28
1	A	614	HIS	CB-CG-CD2	-7.76	121.11	131.20
1	A	321	PRO	CA-C-N	-7.71	115.29	123.08
1	A	321	PRO	C-N-CA	-7.71	115.29	123.08
1	A	557	ILE	N-CA-C	-7.69	98.37	109.29
1	A	95	LEU	N-CA-C	7.67	120.37	111.02
1	A	575	ARG	N-CA-C	7.60	122.00	111.74
1	A	61	ASP	CA-CB-CG	7.55	120.15	112.60
1	A	282	ASN	CA-C-N	7.48	134.23	122.26
1	A	282	ASN	C-N-CA	7.48	134.23	122.26
1	A	169	LYS	N-CA-C	-7.43	96.83	109.24
1	A	80	LYS	N-CA-C	-7.42	98.83	109.96
1	A	563	PHE	N-CA-C	-7.41	95.54	108.20
1	A	87	LEU	N-CA-C	-7.40	103.85	113.17
1	A	598	VAL	N-CA-C	-7.36	97.90	108.42
1	A	676	THR	CB-CA-C	7.35	121.37	109.02
1	A	686	ALA	N-CA-C	-7.33	98.16	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ILE	N-CA-CB	-7.25	99.27	111.23
1	A	41	LYS	N-CA-C	-7.23	98.37	109.14
1	A	726	TYR	N-CA-C	-7.22	98.79	110.20
1	A	163	PHE	N-CA-C	-7.12	97.34	109.24
1	A	14	SER	CB-CA-C	-7.10	96.62	110.10
1	A	324	THR	CA-C-N	-7.07	110.21	122.37
1	A	324	THR	C-N-CA	-7.07	110.21	122.37
1	A	187	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	A	436	VAL	N-CA-C	-7.06	96.06	107.28
1	A	633	ASP	N-CA-C	-7.04	100.92	109.72
1	A	784	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	A	767	HIS	CB-CG-CD2	-6.98	122.13	131.20
1	A	241	MET	N-CA-C	-6.96	97.06	108.41
1	A	467	ILE	N-CA-C	6.95	117.74	110.72
1	A	430	LEU	N-CA-C	-6.93	104.79	113.18
1	A	689	ILE	N-CA-C	-6.89	98.52	108.17
1	A	115	LEU	N-CA-C	-6.89	104.69	113.23
1	A	291	LEU	N-CA-C	-6.87	104.38	112.89
1	A	520	LYS	N-CA-C	-6.86	104.78	113.01
1	A	724	ARG	CA-CB-CG	6.86	127.83	114.10
1	A	636	VAL	N-CA-C	-6.86	105.16	111.67
1	A	205	ARG	N-CA-C	-6.82	98.98	109.14
1	A	494	LEU	O-C-N	-6.79	113.13	122.30
1	A	36	HIS	CB-CG-CD2	-6.74	122.44	131.20
1	A	200	VAL	N-CA-C	-6.73	98.43	108.46
1	A	478	LYS	N-CA-CB	-6.71	99.97	110.44
1	A	584	ILE	CA-CB-CG2	-6.71	99.10	110.50
1	A	260	GLY	N-CA-C	-6.70	97.30	113.18
1	A	349	LEU	N-CA-C	-6.69	104.07	111.36
1	A	214	LYS	N-CA-C	-6.69	98.07	109.24
1	A	571	HIS	CB-CG-ND1	6.64	132.66	122.70
1	A	733	ASP	O-C-N	-6.64	114.58	122.15
1	A	129	ALA	N-CA-C	-6.62	96.34	107.99
1	A	15	VAL	CA-C-N	6.60	133.16	122.67
1	A	15	VAL	C-N-CA	6.60	133.16	122.67
1	A	73	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	16	ARG	CD-NE-CZ	6.55	133.57	124.40
1	A	287	GLU	N-CA-C	-6.54	97.41	108.26
1	A	807	THR	CB-CA-C	6.54	121.01	110.09
1	A	237	VAL	N-CA-C	-6.53	98.98	108.71
1	A	681	PHE	CA-CB-CG	6.53	120.33	113.80
1	A	614	HIS	CB-CG-ND1	6.51	132.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	VAL	N-CA-C	-6.50	99.00	108.11
1	A	584	ILE	CA-CB-CG1	6.50	121.45	110.40
1	A	171	CYS	N-CA-C	-6.50	97.48	108.26
1	A	42	ASP	O-C-N	-6.49	115.74	123.27
1	A	456	ALA	N-CA-C	-6.48	98.52	108.76
1	A	558	ASN	N-CA-C	-6.44	100.28	109.62
1	A	454	GLY	N-CA-C	-6.43	101.52	112.51
1	A	261	GLY	N-CA-C	-6.42	97.96	113.18
1	A	61	ASP	O-C-N	-6.42	115.32	122.12
1	A	241	MET	CA-C-O	-6.42	113.44	120.30
1	A	696	ASN	N-CA-C	-6.39	104.74	112.54
1	A	519	ARG	CA-CB-CG	6.39	126.88	114.10
1	A	222	LEU	N-CA-C	-6.37	99.82	109.95
1	A	597	PHE	N-CA-C	-6.34	101.09	110.48
1	A	246	ALA	N-CA-C	-6.33	99.98	110.17
1	A	152	LEU	N-CA-C	-6.29	100.04	110.17
1	A	142	CYS	N-CA-C	-6.27	104.54	111.82
1	A	641	ARG	N-CA-C	-6.27	97.59	108.69
1	A	811	PHE	CA-CB-CG	-6.26	107.53	113.80
1	A	81	ARG	N-CA-C	-6.26	100.72	110.42
1	A	125	ILE	N-CA-C	-6.26	105.52	113.22
1	A	223	ALA	N-CA-C	-6.25	98.71	108.90
1	A	232	GLY	N-CA-C	-6.25	104.19	112.82
1	A	605	ILE	N-CA-C	-6.23	99.18	108.46
1	A	837	PRO	N-CA-C	-6.22	99.66	112.47
1	A	360	ASP	N-CA-C	-6.21	100.39	110.20
1	A	63	LEU	N-CA-C	-6.18	105.53	114.12
1	A	150	LEU	N-CA-C	-6.18	105.06	112.59
1	A	41	LYS	CA-C-N	6.13	132.41	122.29
1	A	41	LYS	C-N-CA	6.13	132.41	122.29
1	A	80	LYS	CA-C-O	-6.11	113.79	120.81
1	A	254	LEU	O-C-N	-6.10	116.02	122.30
1	A	391	LEU	N-CA-C	-6.08	104.21	111.69
1	A	230	VAL	CA-C-O	-6.08	116.75	120.88
1	A	451	ALA	N-CA-C	-6.06	99.83	109.23
1	A	238	VAL	N-CA-C	-6.05	98.76	107.78
1	A	41	LYS	O-C-N	-6.05	115.34	122.96
1	A	341	HIS	O-C-N	-6.05	114.99	120.92
1	A	675	GLY	N-CA-C	-6.05	98.85	113.18
1	A	611	PRO	O-C-N	-6.04	115.22	122.89
1	A	309	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	A	164	GLY	N-CA-C	-6.01	103.89	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	PHE	N-CA-C	-6.01	104.65	111.14
1	A	334	ALA	N-CA-C	-6.01	98.06	108.69
1	A	235	ASN	CA-CB-CG	6.00	118.60	112.60
1	A	386	ARG	O-C-N	-6.00	116.25	123.27
1	A	216	VAL	N-CA-CB	-6.00	104.12	112.52
1	A	366	GLU	CA-CB-CG	5.98	126.06	114.10
1	A	455	VAL	O-C-N	-5.97	115.97	122.05
1	A	632	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	771	PHE	CA-CB-CG	-5.96	107.84	113.80
1	A	380	ILE	N-CA-CB	-5.96	102.86	111.21
1	A	15	VAL	CA-CB-CG1	-5.92	100.33	110.40
1	A	85	LEU	O-C-N	-5.92	116.47	123.22
1	A	379	VAL	N-CA-C	-5.92	106.98	113.43
1	A	579	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	575	ARG	CB-CG-CD	-5.88	97.78	111.30
1	A	320	ASP	O-C-N	-5.87	114.56	121.32
1	A	676	THR	N-CA-C	-5.85	106.76	114.31
1	A	585	THR	N-CA-C	-5.83	104.93	111.28
1	A	582	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	A	335	ILE	N-CA-C	-5.81	99.81	108.46
1	A	714	ARG	N-CA-C	-5.78	100.86	109.94
1	A	308	ILE	CA-C-N	5.77	128.32	120.54
1	A	308	ILE	C-N-CA	5.77	128.32	120.54
1	A	467	ILE	CA-C-N	-5.76	114.04	122.86
1	A	467	ILE	C-N-CA	-5.76	114.04	122.86
1	A	455	VAL	N-CA-CB	-5.76	105.65	112.39
1	A	57	HIS	O-C-N	-5.74	114.73	122.43
1	A	148	ALA	N-CA-C	-5.72	104.42	111.40
1	A	602	THR	N-CA-C	-5.71	97.88	107.99
1	A	94	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	828	GLU	CA-C-N	5.68	125.69	119.89
1	A	828	GLU	C-N-CA	5.68	125.69	119.89
1	A	78	ASP	N-CA-C	5.64	122.28	109.81
1	A	513	SER	N-CA-C	-5.64	103.77	111.56
1	A	224	MET	CA-C-O	-5.63	114.14	119.55
1	A	211	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	A	390	HIS	CA-CB-CG	5.60	119.40	113.80
1	A	798	THR	CA-CB-OG1	-5.60	101.21	109.60
1	A	667	SER	CA-CB-OG	-5.59	99.91	111.10
1	A	836	ALA	N-CA-C	5.58	122.15	109.81
1	A	455	VAL	N-CA-C	5.58	116.87	111.91
1	A	816	THR	CA-CB-OG1	-5.57	101.24	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	A	829	PRO	N-CA-C	5.56	119.95	111.11
1	A	292	ARG	CA-CB-CG	-5.53	103.04	114.10
1	A	757	LEU	O-C-N	-5.53	115.52	122.20
1	A	560	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	37	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	184	ARG	CA-CB-CG	5.49	125.09	114.10
1	A	825	TRP	CG-CD2-CE3	5.49	139.39	133.90
1	A	638	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	184	ARG	N-CA-C	5.47	117.95	111.33
1	A	247	LYS	N-CA-C	-5.47	99.75	109.06
1	A	798	THR	N-CA-CB	-5.47	101.80	110.22
1	A	467	ILE	CB-CA-C	-5.46	104.69	112.22
1	A	63	LEU	N-CA-CB	-5.46	103.35	110.88
1	A	298	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	86	SER	N-CA-C	-5.45	101.01	109.24
1	A	764	MET	CA-CB-CG	5.45	125.00	114.10
1	A	375	THR	CA-CB-OG1	-5.45	101.43	109.60
1	A	118	ASP	CA-C-O	5.44	128.29	120.51
1	A	167	ASN	N-CA-C	-5.44	100.37	109.24
1	A	117	LEU	N-CA-C	5.43	121.46	114.56
1	A	725	GLY	N-CA-C	-5.43	100.31	113.18
1	A	335	ILE	CB-CG1-CD1	-5.43	102.40	113.80
1	A	529	ALA	N-CA-C	-5.42	105.02	111.69
1	A	555	VAL	N-CA-CB	-5.42	102.28	111.23
1	A	471	PHE	N-CA-C	-5.42	105.40	112.23
1	A	784	GLN	CG-CD-NE2	5.41	124.52	116.40
1	A	149	THR	CA-CB-OG1	-5.41	101.49	109.60
1	A	677	GLY	O-C-N	5.41	127.38	122.19
1	A	519	ARG	CB-CG-CD	-5.40	98.88	111.30
1	A	53	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	360	ASP	CA-CB-CG	-5.40	107.20	112.60
1	A	162	GLU	N-CA-C	-5.39	105.57	111.82
1	A	565	VAL	N-CA-C	5.38	116.42	108.45
1	A	827	VAL	N-CA-C	-5.38	100.09	108.86
1	A	555	VAL	N-CA-C	5.36	120.49	109.34
1	A	296	GLU	O-C-N	-5.34	116.45	122.12
1	A	319	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	230	VAL	CA-C-N	5.33	126.15	120.13
1	A	230	VAL	C-N-CA	5.33	126.15	120.13
1	A	581	LEU	N-CA-C	-5.33	105.64	111.82
1	A	155	TYR	N-CA-C	-5.33	100.00	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	N-CA-C	-5.32	101.64	109.62
1	A	320	ASP	CA-C-N	5.32	126.49	119.84
1	A	320	ASP	C-N-CA	5.32	126.49	119.84
1	A	156	GLY	N-CA-C	-5.31	102.58	110.71
1	A	624	THR	N-CA-C	-5.31	105.66	111.82
1	A	286	PHE	CA-C-N	-5.31	114.53	122.39
1	A	286	PHE	C-N-CA	-5.31	114.53	122.39
1	A	526	ASP	N-CA-C	-5.31	106.03	112.88
1	A	399	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	315	LYS	N-CA-CB	-5.29	101.54	110.49
1	A	672	GLU	N-CA-C	-5.29	101.07	109.96
1	A	745	LEU	N-CA-C	-5.29	105.41	111.07
1	A	774	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	437	LYS	N-CA-C	-5.29	102.03	109.96
1	A	599	VAL	CA-C-N	5.29	125.21	119.76
1	A	599	VAL	C-N-CA	5.29	125.21	119.76
1	A	54	ALA	CA-C-N	-5.28	111.55	120.58
1	A	54	ALA	C-N-CA	-5.28	111.55	120.58
1	A	198	LEU	N-CA-C	-5.28	100.98	109.58
1	A	783	CYS	N-CA-C	-5.26	105.63	111.36
1	A	459	HIS	N-CA-C	-5.25	105.73	111.82
1	A	683	LEU	O-C-N	-5.25	115.69	122.20
1	A	145	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	284	ASN	CA-C-N	5.22	131.51	121.54
1	A	284	ASN	C-N-CA	5.22	131.51	121.54
1	A	413	ARG	N-CA-C	-5.21	105.68	111.36
1	A	579	ASN	CB-CG-ND2	5.21	124.21	116.40
1	A	632	HIS	N-CA-C	-5.20	105.64	112.41
1	A	678	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	782	LYS	CA-CB-CG	-5.20	103.70	114.10
1	A	424	ARG	N-CA-C	-5.20	105.51	111.07
1	A	20	GLY	O-C-N	5.18	129.44	122.70
1	A	742	ILE	N-CA-C	-5.18	105.49	110.72
1	A	720	ARG	N-CA-C	-5.17	105.72	111.36
1	A	727	ASN	CA-CB-CG	-5.17	107.43	112.60
1	A	475	GLU	CA-C-N	5.16	124.78	119.05
1	A	475	GLU	C-N-CA	5.16	124.78	119.05
1	A	688	THR	CA-C-N	-5.16	116.79	123.19
1	A	688	THR	C-N-CA	-5.16	116.79	123.19
1	A	693	ASP	N-CA-C	-5.16	101.45	109.24
1	A	18	LEU	CB-CG-CD1	-5.13	95.30	110.70
1	A	394	THR	N-CA-C	5.13	116.56	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	807	THR	O-C-N	-5.13	115.92	122.34
1	A	245	SER	N-CA-C	-5.12	101.41	109.50
1	A	785	GLU	N-CA-C	-5.12	105.88	111.82
1	A	632	HIS	CA-CB-CG	-5.11	108.69	113.80
1	A	323	ARG	CA-CB-CG	5.11	124.31	114.10
1	A	749	PHE	N-CA-C	-5.09	105.81	111.36
1	A	797	TRP	N-CA-C	-5.09	105.64	111.14
1	A	495	CYS	O-C-N	-5.08	115.44	122.46
1	A	674	SER	N-CA-C	-5.07	99.99	110.80
1	A	226	TYR	CA-C-O	-5.05	114.71	120.32
1	A	170	ILE	N-CA-C	-5.05	101.21	108.53
1	A	62	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	A	319	ARG	CA-CB-CG	-5.05	104.01	114.10
1	A	768	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	A	789	ALA	N-CA-C	-5.05	105.67	111.07
1	A	339	ASP	O-C-N	-5.04	115.88	122.59
1	A	390	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	A	715	VAL	CA-C-O	-5.04	115.82	121.17
1	A	52	TYR	N-CA-C	-5.04	105.68	111.07
1	A	372	CYS	N-CA-C	5.03	118.33	110.32
1	A	483	THR	CA-CB-OG1	-5.03	102.05	109.60
1	A	220	VAL	O-C-N	-5.03	118.01	123.14
1	A	319	ARG	N-CA-C	-5.02	100.89	108.67
1	A	334	ALA	O-C-N	-5.02	117.24	123.36
1	A	576	GLN	N-CA-C	-5.02	105.94	111.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	19	ALA	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	SER	Mainchain
1	A	15	VAL	Mainchain
1	A	16	ARG	Sidechain
1	A	18	LEU	Peptide
1	A	286	PHE	Mainchain
1	A	320	ASP	Peptide
1	A	57	HIS	Sidechain,Mainchain
1	A	836	ALA	Peptide

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	6727	0	6654	211	1
2	B	56	0	48	12	0
3	A	17	0	13	9	0
4	A	15	0	7	2	0
5	A	46	0	22	1	0
6	A	608	0	0	27	1
All	All	7469	0	6744	220	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 16.

All (220) 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:14:SER:CA	1:A:14:SER:CB	1.76	1.57
1:A:18:LEU:CD2	1:A:18:LEU:CG	1.84	1.51
1:A:332:LYS:CE	1:A:332:LYS:NZ	1.74	1.46
1:A:15:VAL:CA	1:A:15:VAL:C	1.86	1.45
1:A:18:LEU:C	1:A:18:LEU:CA	2.00	1.35
1:A:18:LEU:CD2	6:A:1376:HOH:O	1.86	1.19
1:A:309:ARG:HG2	1:A:309:ARG:NH1	1.53	1.10
1:A:15:VAL:CA	1:A:16:ARG:N	2.17	1.08
1:A:57:HIS:CE1	6:A:1431:HOH:O	2.09	1.06
1:A:18:LEU:CG	6:A:1376:HOH:O	2.03	1.05
1:A:309:ARG:HH11	1:A:309:ARG:CG	1.69	1.04
1:A:309:ARG:NE	6:A:1249:HOH:O	1.85	1.02
1:A:14:SER:CB	1:A:14:SER:C	2.33	1.01
1:A:18:LEU:CD1	6:A:1376:HOH:O	2.14	0.95
1:A:14:SER:HB2	1:A:16:ARG:HG2	1.49	0.94
1:A:312:LYS:NZ	1:A:357:GLU:OE2	2.01	0.94
1:A:15:VAL:HG23	6:A:1160:HOH:O	1.66	0.94
1:A:286:PHE:CD1	1:A:286:PHE:C	2.46	0.93
1:A:312:LYS:NZ	1:A:312:LYS:CE	2.35	0.90
1:A:309:ARG:O	1:A:309:ARG:C	2.16	0.89
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.58	0.85
1:A:15:VAL:CA	1:A:16:ARG:H	1.88	0.84
1:A:426:ARG:HB2	2:B:1:GLC:O2	1.78	0.83
1:A:19:ALA:HB2	1:A:106:ASN:O	1.79	0.83
1:A:332:LYS:NZ	1:A:332:LYS:CD	2.45	0.78
2:B:1:GLC:O3	2:B:2:GLC:C1	2.31	0.78
1:A:309:ARG:CD	6:A:1249:HOH:O	2.25	0.78
2:B:2:GLC:C4	2:B:3:GLC:C1	2.62	0.77
1:A:18:LEU:CD2	1:A:18:LEU:CB	2.58	0.77
3:A:998:H2P:O2	3:A:998:H2P:OP3	2.02	0.77
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.70	0.73
1:A:309:ARG:HG2	1:A:309:ARG:HH11	0.74	0.73
1:A:283:ASP:HB3	1:A:569:ARG:HD2	1.71	0.72
1:A:314:SER:C	1:A:316:PHE:H	1.97	0.72
1:A:569:ARG:NH1	3:A:998:H2P:P	2.64	0.70
1:A:312:LYS:NZ	1:A:357:GLU:CD	2.50	0.70
1:A:315:LYS:C	1:A:317:GLY:H	1.98	0.69
1:A:312:LYS:HZ2	1:A:357:GLU:CD	1.99	0.69
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.75	0.68
1:A:730:GLU:O	1:A:734:ARG:HG2	1.93	0.68
1:A:15:VAL:C	1:A:15:VAL:CB	2.66	0.68
1:A:99:MET:HE2	1:A:105:GLU:HA	1.77	0.66
1:A:316:PHE:CD1	1:A:319:ARG:HD3	2.30	0.66
1:A:282:ASN:ND2	1:A:285:PHE:HD2	1.94	0.66
1:A:166:PHE:O	1:A:608:LYS:HE2	1.96	0.66
1:A:426:ARG:HB2	2:B:1:GLC:HO2	1.59	0.65
1:A:16:ARG:NH1	1:A:105:GLU:OE2	2.30	0.65
1:A:312:LYS:NZ	1:A:357:GLU:OE1	2.30	0.65
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.79	0.64
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.79	0.64
1:A:569:ARG:NH1	3:A:998:H2P:OP3	2.30	0.64
1:A:18:LEU:HD21	6:A:1376:HOH:O	1.68	0.63
1:A:309:ARG:O	1:A:313:SER:N	2.31	0.63
1:A:316:PHE:CE1	1:A:319:ARG:HD3	2.34	0.63
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.34	0.63
1:A:99:MET:HE1	1:A:119:MET:SD	2.38	0.62
3:A:998:H2P:OP1	3:A:998:H2P:H3	2.01	0.61
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.64	0.60
1:A:320:ASP:HB3	1:A:321:PRO:HD3	1.83	0.60
1:A:15:VAL:HA	1:A:16:ARG:H	1.66	0.60
1:A:665:GLN:HG2	1:A:678:ASN:HD22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HG23	1:A:711:PHE:HZ	1.67	0.60
1:A:18:LEU:O	6:A:1576:HOH:O	2.15	0.60
1:A:665:GLN:HG2	1:A:678:ASN:ND2	2.16	0.59
1:A:18:LEU:C	1:A:18:LEU:CB	2.75	0.59
1:A:263:ILE:O	1:A:267:LEU:HG	2.02	0.59
1:A:584:ILE:HG21	1:A:750:PHE:CZ	2.38	0.59
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.84	0.59
1:A:790:LEU:HD12	1:A:797:TRP:HD1	1.68	0.58
1:A:569:ARG:NH1	3:A:998:H2P:OP2	2.34	0.58
1:A:314:SER:C	1:A:316:PHE:N	2.60	0.58
1:A:584:ILE:HG21	1:A:750:PHE:HZ	1.68	0.57
1:A:314:SER:O	1:A:316:PHE:N	2.27	0.57
1:A:378:THR:HG22	1:A:380:ILE:HB	1.87	0.57
1:A:589:ARG:HH11	1:A:589:ARG:HG3	1.69	0.57
1:A:549:LEU:HB3	1:A:555:VAL:HG11	1.86	0.56
1:A:21:VAL:HG13	1:A:22:GLU:N	2.20	0.56
1:A:424:ARG:HH22	1:A:473:GLU:CD	2.13	0.56
1:A:424:ARG:HH21	1:A:470:ASP:HA	1.71	0.56
1:A:15:VAL:HB	1:A:509:GLU:OE2	2.04	0.56
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.88	0.56
1:A:408:GLN:HE21	2:B:4:GLC:H61	1.71	0.56
1:A:16:ARG:NH1	6:A:1419:HOH:O	2.35	0.56
1:A:49:ARG:HD2	6:A:1566:HOH:O	2.06	0.55
1:A:343:SER:HB3	1:A:445:CYS:SG	2.46	0.55
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.06	0.55
1:A:250:ASN:HA	1:A:269:ARG:NH1	2.22	0.55
3:A:998:H2P:P	3:A:998:H2P:HO2	2.30	0.55
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.72	0.54
1:A:742:ILE:HG21	1:A:766:MET:HE3	1.89	0.54
1:A:432:GLU:HB3	1:A:438:ARG:HG3	1.90	0.54
1:A:143:PHE:HB3	1:A:147:MET:HE3	1.90	0.54
1:A:225:PRO:CB	1:A:242:ARG:HD2	2.33	0.54
1:A:428:MET:SD	1:A:470:ASP:HB3	2.48	0.53
1:A:392:LEU:HD13	1:A:439:ILE:HD12	1.90	0.53
1:A:286:PHE:C	1:A:286:PHE:HD1	2.10	0.53
1:A:810:LYS:NZ	6:A:1450:HOH:O	2.41	0.53
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.08	0.53
2:B:2:GLC:O4	2:B:3:GLC:O5	2.21	0.53
3:A:998:H2P:OP1	4:A:999:PLP:O3P	2.26	0.53
1:A:320:ASP:HB3	1:A:321:PRO:CD	2.37	0.53
1:A:15:VAL:C	1:A:15:VAL:N	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD23	1:A:55:LEU:O	2.09	0.52
1:A:204:GLY:HA2	1:A:217:ASP:O	2.08	0.52
1:A:792:LYS:O	1:A:794:PRO:HD3	2.10	0.52
1:A:283:ASP:HB3	1:A:569:ARG:CD	2.39	0.52
1:A:569:ARG:HH11	3:A:998:H2P:P	2.30	0.52
1:A:102:LEU:HB3	1:A:104:LEU:HD23	1.91	0.52
1:A:408:GLN:HG3	2:B:4:GLC:H61	1.92	0.52
1:A:375:THR:HG23	1:A:453:ASN:HD21	1.76	0.51
1:A:433:GLU:CD	2:B:3:GLC:HO2	2.18	0.51
1:A:737:GLU:O	1:A:740:GLN:HG2	2.11	0.51
1:A:568:LYS:O	1:A:607:GLY:HA3	2.11	0.51
1:A:285:PHE:HA	1:A:383:ALA:HA	1.92	0.50
1:A:455:VAL:H	1:A:459:HIS:HD2	1.59	0.50
1:A:555:VAL:HG13	1:A:557:ILE:HG23	1.93	0.50
1:A:803:ARG:O	1:A:807:THR:HB	2.11	0.50
1:A:469:LYS:NZ	6:A:1168:HOH:O	2.45	0.50
1:A:315:LYS:C	1:A:317:GLY:N	2.70	0.49
1:A:399:HIS:O	1:A:403:ILE:HG13	2.12	0.49
1:A:441:MET:HE3	1:A:444:LEU:HD12	1.93	0.49
1:A:55:LEU:HD23	1:A:59:VAL:HG23	1.94	0.49
1:A:380:ILE:HA	1:A:381:PRO:HD3	1.67	0.49
1:A:490:ARG:HA	1:A:494:LEU:HB3	1.94	0.49
1:A:422:VAL:HG12	2:B:1:GLC:H2	1.94	0.48
1:A:707:ASN:HA	1:A:800:MET:SD	2.53	0.48
1:A:142:CYS:SG	1:A:487:THR:HG22	2.53	0.48
1:A:474:LEU:HD12	1:A:475:GLU:HG3	1.95	0.48
1:A:289:LYS:NZ	6:A:1557:HOH:O	2.47	0.48
1:A:678:ASN:HB3	1:A:699:MET:SD	2.54	0.48
1:A:315:LYS:N	1:A:315:LYS:HD2	2.28	0.48
1:A:208:HIS:HB2	6:A:1264:HOH:O	2.12	0.48
1:A:538:LYS:HA	1:A:538:LYS:HD2	1.68	0.47
1:A:282:ASN:HD21	1:A:285:PHE:HD2	1.62	0.47
3:A:998:H2P:P	3:A:998:H2P:H3	2.54	0.47
1:A:63:LEU:HD21	1:A:229:PRO:HG3	1.96	0.47
1:A:18:LEU:CG	1:A:18:LEU:CD1	2.93	0.47
1:A:93:ARG:HD3	1:A:126:GLU:O	2.14	0.47
1:A:402:ILE:O	1:A:406:ILE:HG12	2.15	0.47
1:A:764:MET:SD	1:A:765:LEU:HD13	2.54	0.47
1:A:301:ALA:O	1:A:305:GLN:HG3	2.14	0.47
1:A:705:GLU:HG2	1:A:710:ILE:HD12	1.97	0.47
1:A:41:LYS:NZ	6:A:1565:HOH:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:PHE:HB3	1:A:686:ALA:HB3	1.97	0.47
1:A:82:ILE:HD13	1:A:825:TRP:CE3	2.50	0.46
1:A:335:ILE:HD13	1:A:335:ILE:HG21	1.51	0.46
1:A:354:VAL:O	1:A:358:ARG:HA	2.15	0.46
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.49	0.46
1:A:378:THR:HG22	1:A:380:ILE:H	1.79	0.46
1:A:389:VAL:HG23	1:A:400:LEU:HD21	1.97	0.46
1:A:759:LYS:NZ	6:A:1535:HOH:O	2.47	0.46
1:A:723:GLN:HB2	6:A:1528:HOH:O	2.15	0.46
1:A:455:VAL:HB	1:A:484:ASN:ND2	2.31	0.46
1:A:579:ASN:HB2	6:A:1332:HOH:O	2.16	0.46
1:A:23:ASN:HA	1:A:26:GLU:HG2	1.96	0.45
1:A:14:SER:CB	1:A:14:SER:HA	2.18	0.45
1:A:375:THR:HG23	1:A:453:ASN:ND2	2.31	0.45
1:A:589:ARG:HH12	1:A:737:GLU:CD	2.24	0.45
1:A:175:GLN:HG2	1:A:177:GLU:OE1	2.17	0.45
1:A:392:LEU:HB3	1:A:400:LEU:HG	1.98	0.45
1:A:532:ARG:HH11	1:A:532:ARG:HD3	1.66	0.45
1:A:488:PRO:O	1:A:492:LEU:HB3	2.17	0.45
1:A:309:ARG:NH1	1:A:309:ARG:CG	2.39	0.45
1:A:426:ARG:NH2	6:A:1182:HOH:O	2.47	0.44
1:A:332:LYS:NZ	1:A:332:LYS:HD3	2.29	0.44
1:A:169:LYS:NZ	6:A:1029:HOH:O	2.50	0.44
1:A:676:THR:HG22	4:A:999:PLP:H5A1	1.98	0.44
1:A:93:ARG:HD2	1:A:126:GLU:HB3	1.99	0.44
1:A:21:VAL:CG1	1:A:22:GLU:N	2.80	0.44
2:B:1:GLC:H3	2:B:2:GLC:O2	2.17	0.44
1:A:55:LEU:HD13	1:A:119:MET:CE	2.48	0.43
1:A:517:GLN:OE1	1:A:520:LYS:NZ	2.52	0.43
1:A:522:LEU:HD12	1:A:522:LEU:HA	1.78	0.43
1:A:721:LEU:HD23	1:A:772:LYS:HD3	2.00	0.43
1:A:358:ARG:HD3	6:A:1597:HOH:O	2.18	0.43
1:A:418:PHE:HE2	1:A:474:LEU:HD23	1.82	0.43
1:A:408:GLN:CG	2:B:4:GLC:H61	2.48	0.43
1:A:469:LYS:HD2	6:A:1167:HOH:O	2.16	0.43
1:A:765:LEU:HD12	1:A:765:LEU:HA	1.81	0.43
1:A:817:ILE:HD12	1:A:817:ILE:HA	1.79	0.43
1:A:316:PHE:HD1	1:A:319:ARG:HD3	1.81	0.43
1:A:177:GLU:CD	1:A:617:LYS:HZ3	2.26	0.43
1:A:457:ARG:HG3	1:A:458:ILE:N	2.34	0.42
1:A:386:ARG:NH2	6:A:1181:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:HB2	1:A:324:THR:H	1.53	0.42
1:A:389:VAL:HG22	1:A:400:LEU:HD11	2.01	0.42
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.82	0.42
1:A:666:ILE:HD13	1:A:780:TYR:CE1	2.55	0.42
1:A:703:ALA:CA	1:A:807:THR:HG21	2.50	0.42
1:A:665:GLN:C	1:A:666:ILE:HG13	2.45	0.42
1:A:282:ASN:ND2	1:A:285:PHE:CD2	2.82	0.41
1:A:365:TRP:CZ3	1:A:406:ILE:HD12	2.55	0.41
1:A:253:ASN:O	1:A:265:ALA:HB1	2.19	0.41
1:A:423:ASP:O	1:A:426:ARG:HB3	2.21	0.41
1:A:319:ARG:NH2	6:A:1275:HOH:O	2.53	0.41
1:A:408:GLN:CG	2:B:4:GLC:C6	2.99	0.41
1:A:592:LYS:HA	1:A:592:LYS:HD2	1.89	0.41
1:A:374:TYR:HD2	1:A:452:VAL:HG13	1.86	0.41
1:A:400:LEU:HD23	1:A:400:LEU:HA	1.86	0.41
1:A:591:LYS:NZ	6:A:1099:HOH:O	2.54	0.41
1:A:753:LYS:HD2	1:A:753:LYS:H	1.86	0.41
1:A:304:LEU:O	1:A:308:ILE:HG12	2.20	0.41
1:A:613:TYR:CZ	5:A:913:AMP:H3'	2.55	0.41
1:A:821:ALA:O	1:A:826:GLY:N	2.53	0.41
1:A:832:GLN:HG3	6:A:1037:HOH:O	2.21	0.41
1:A:309:ARG:O	1:A:313:SER:CB	2.69	0.41
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.88	0.41
1:A:98:THR:O	1:A:102:LEU:HB2	2.21	0.41
1:A:325:ASN:HD22	1:A:325:ASN:HA	1.61	0.41
1:A:486:ILE:HD11	1:A:680:LYS:HE3	2.03	0.41
1:A:487:THR:HA	1:A:488:PRO:HD2	1.87	0.41
1:A:585:THR:OG1	1:A:741:ILE:HD11	2.20	0.41
1:A:742:ILE:HD13	1:A:742:ILE:HA	1.86	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD2	1.79	0.41
1:A:340:THR:HG23	1:A:374:TYR:CE1	2.55	0.41
1:A:683:LEU:O	1:A:684:ASN:HB2	2.21	0.40
1:A:93:ARG:HB3	1:A:126:GLU:OE1	2.21	0.40
1:A:25:THR:HA	1:A:28:LYS:HE2	2.01	0.40
1:A:291:LEU:O	1:A:295:GLN:HG3	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:ARG:NH1	6:A:1229:HOH:O[5_545]	1.79	0.41

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	826/842 (98%)	766 (93%)	44 (5%)	16 (2%)	6	14

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	284	ASN
1	A	320	ASP
1	A	323	ARG
1	A	315	LYS
1	A	435	ALA
1	A	556	HIS
1	A	837	PRO
1	A	21	VAL
1	A	118	ASP
1	A	210	SER
1	A	555	VAL
1	A	256	ASP
1	A	678	ASN
1	A	514	ASP
1	A	342	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	715/731 (98%)	619 (87%)	96 (13%)	4 7

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	26	GLU
1	A	27	LEU
1	A	29	LYS
1	A	44	ASN
1	A	57	HIS
1	A	60	ARG
1	A	63	LEU
1	A	80	LYS
1	A	85	LEU
1	A	93	ARG
1	A	102	LEU
1	A	106	ASN
1	A	112	THR
1	A	115	LEU
1	A	119	MET
1	A	127	GLU
1	A	131	LEU
1	A	136	LEU
1	A	138	ARG
1	A	144	LEU
1	A	152	LEU
1	A	165	ILE
1	A	170	ILE
1	A	177	GLU
1	A	198	LEU
1	A	211	GLN
1	A	234	ARG
1	A	235	ASN
1	A	242	ARG
1	A	243	LEU
1	A	245	SER
1	A	264	GLN
1	A	284	ASN
1	A	286	PHE

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Mol	Chain	Res	Type
1	A	309	ARG
1	A	315	LYS
1	A	325	ASN
1	A	337	LEU
1	A	340	THR
1	A	344	LEU
1	A	375	THR
1	A	380	ILE
1	A	386	ARG
1	A	392	LEU
1	A	398	ARG
1	A	400	LEU
1	A	413	ARG
1	A	426	ARG
1	A	441	MET
1	A	444	LEU
1	A	466	THR
1	A	474	LEU
1	A	486	ILE
1	A	490	ARG
1	A	502	ILE
1	A	506	ARG
1	A	513	SER
1	A	515	LEU
1	A	521	LEU
1	A	522	LEU
1	A	528	GLU
1	A	549	LEU
1	A	555	VAL
1	A	560	ASN
1	A	565	VAL
1	A	568	LYS
1	A	576	GLN
1	A	584	ILE
1	A	589	ARG
1	A	593	GLU
1	A	622	LEU
1	A	624	THR
1	A	645	LEU
1	A	649	ARG
1	A	662	LEU
1	A	665	GLN

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Mol	Chain	Res	Type
1	A	667	SER
1	A	676	THR
1	A	687	LEU
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	720	ARG
1	A	751	SER
1	A	753	LYS
1	A	763	ASN
1	A	765	LEU
1	A	790	LEU
1	A	795	ARG
1	A	797	TRP
1	A	807	THR
1	A	808	SER
1	A	813	SER
1	A	817	ILE
1	A	839	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	264	GLN
1	A	325	ASN
1	A	453	ASN
1	A	481	ASN
1	A	484	ASN
1	A	496	ASN
1	A	541	ASN
1	A	576	GLN
1	A	678	ASN
1	A	696	ASN
1	A	740	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 ⓘ

5 monosaccharides 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	B	1	2	12,12,12	1.09	1 (8%)	17,17,17	1.72	2 (11%)
2	GLC	B	2	2	11,11,12	0.56	0	15,15,17	0.84	0
2	GLC	B	3	2	11,11,12	1.87	1 (9%)	15,15,17	1.31	2 (13%)
2	GLC	B	4	2	11,11,12	0.77	0	15,15,17	0.93	1 (6%)
2	GLC	B	5	2	11,11,12	0.47	0	15,15,17	0.86	0

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	B	1	2	-	2/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	0/2/19/22	0/1/1/1
2	GLC	B	4	2	-	0/2/19/22	0/1/1/1
2	GLC	B	5	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	GLC	O5-C1	-5.92	1.33	1.43
2	B	1	GLC	O1-C1	2.57	1.47	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O1-C1-O5	5.40	126.45	110.41
2	B	1	GLC	O3-C3-C2	-3.15	102.95	110.38
2	B	3	GLC	O5-C1-C2	2.81	117.48	110.79
2	B	3	GLC	C1-O5-C5	2.57	115.63	112.19
2	B	4	GLC	C2-C3-C4	-2.22	106.96	110.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

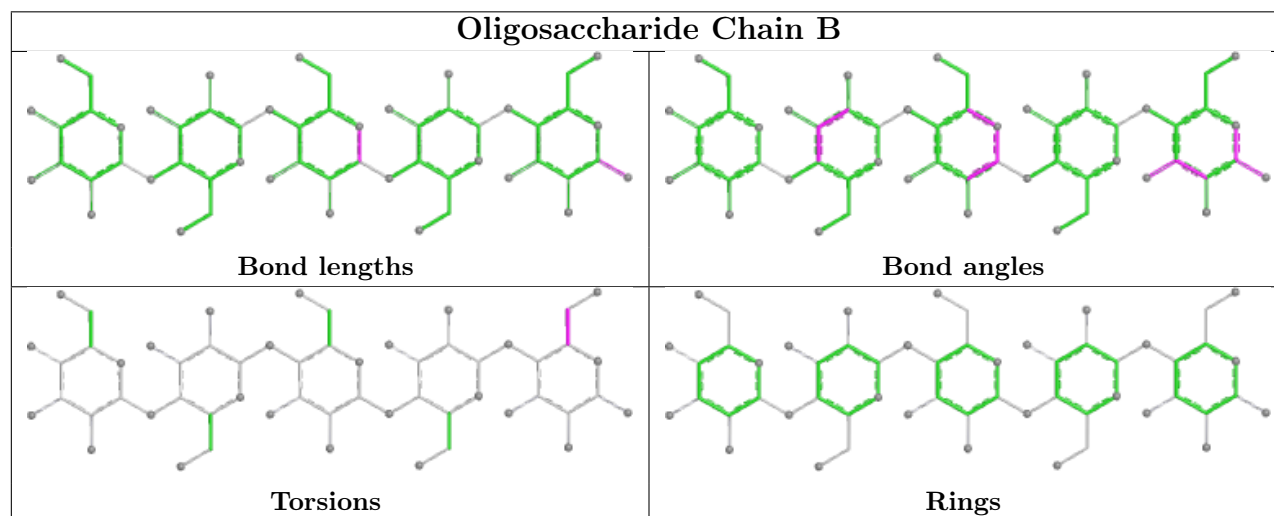
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	GLC	4	0
2	B	1	GLC	5	0
2	B	3	GLC	3	0
2	B	4	GLC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry ⓘ

4 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
5	AMP	A	997	-	25,25,25	1.56	5 (20%)	37,38,38	2.63	21 (56%)
3	H2P	A	998	-	15,17,17	1.75	3 (20%)	20,27,27	1.28	2 (10%)
5	AMP	A	913	-	25,25,25	2.68	7 (28%)	37,38,38	3.11	20 (54%)
4	PLP	A	999	1	15,15,16	1.29	3 (20%)	21,22,23	1.03	1 (4%)

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
5	AMP	A	997	-	-	2/10/26/26	0/3/3/3
3	H2P	A	998	-	-	0/5/31/31	0/1/1/1
5	AMP	A	913	-	-	3/10/26/26	0/3/3/3
4	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	913	AMP	C2-N1	7.65	1.47	1.33
5	A	913	AMP	C8-N7	6.18	1.43	1.31
5	A	913	AMP	O4'-C4'	-5.13	1.33	1.45
5	A	913	AMP	O4'-C1'	4.38	1.52	1.42
5	A	997	AMP	C8-N7	4.24	1.39	1.31
3	A	998	H2P	O5-C1	4.20	1.47	1.42
3	A	998	H2P	P-OP1	2.86	1.59	1.50
5	A	997	AMP	C2-N1	2.75	1.38	1.33
5	A	913	AMP	C2-N3	2.71	1.38	1.33
4	A	999	PLP	C3-C2	-2.58	1.38	1.41
5	A	997	AMP	C2-N3	2.57	1.38	1.33
5	A	997	AMP	C5-C4	-2.51	1.34	1.39
4	A	999	PLP	C5-C4	-2.39	1.37	1.40
5	A	997	AMP	C5-N7	-2.26	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	PLP	C2-N1	2.24	1.37	1.33
5	A	913	AMP	C5-C4	-2.24	1.35	1.39
3	A	998	H2P	O2-C2	2.19	1.47	1.42
5	A	913	AMP	P-O3P	2.03	1.62	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	913	AMP	O4'-C1'-N9	8.15	123.75	108.09
5	A	913	AMP	C6-C5-C4	7.38	127.25	117.18
5	A	913	AMP	C5-C4-N9	6.10	112.45	105.81
5	A	997	AMP	N9-C8-N7	-5.72	105.82	113.94
5	A	913	AMP	O4'-C4'-C3'	5.60	116.27	105.15
5	A	997	AMP	C6-C5-C4	5.28	124.39	117.18
5	A	997	AMP	C5-C4-N3	-5.13	119.65	126.72
5	A	997	AMP	O4'-C1'-N9	4.69	117.10	108.09
5	A	913	AMP	N9-C8-N7	-4.56	107.47	113.94
5	A	913	AMP	C4'-O4'-C1'	-4.31	99.96	109.47
5	A	997	AMP	N3-C2-N1	-4.18	122.26	128.58
5	A	913	AMP	C4-C5-N7	-3.94	106.08	110.58
5	A	913	AMP	O2'-C2'-C1'	3.91	123.56	110.10
5	A	997	AMP	O3'-C3'-C4'	3.84	122.11	111.08
3	A	998	H2P	P-O1-C1	3.52	135.21	127.96
3	A	998	H2P	O5-C1-C7	3.45	108.72	106.06
5	A	997	AMP	C6-C5-N7	-3.39	125.55	132.09
5	A	997	AMP	O4'-C4'-C3'	3.16	111.42	105.15
5	A	913	AMP	C2'-C1'-N9	3.15	121.13	113.30
5	A	913	AMP	C1'-N9-C8	-3.13	120.15	127.09
5	A	997	AMP	C5-N7-C8	2.91	108.02	103.45
5	A	997	AMP	N3-C4-N9	2.91	132.12	127.17
5	A	913	AMP	N3-C2-N1	-2.89	124.21	128.58
5	A	913	AMP	C6-C5-N7	-2.84	126.62	132.09
5	A	913	AMP	N3-C4-N9	-2.79	122.42	127.17
5	A	913	AMP	C2'-C3'-C4'	-2.71	97.37	102.61
5	A	997	AMP	C2'-C1'-N9	2.63	119.84	113.30
5	A	997	AMP	C4'-O4'-C1'	-2.54	103.85	109.47
5	A	997	AMP	N6-C6-N1	2.53	124.01	118.38
5	A	913	AMP	C5-N7-C8	2.50	107.39	103.45
5	A	997	AMP	C2-N3-C4	2.41	117.71	111.83
5	A	913	AMP	O3'-C3'-C2'	2.37	119.42	111.82
5	A	997	AMP	C5'-C4'-C3'	2.36	123.70	115.21
5	A	997	AMP	C4-N9-C1'	-2.29	121.27	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	997	AMP	O2P-P-O1P	2.24	119.56	110.83
5	A	913	AMP	C5-C6-N1	-2.23	111.85	117.51
5	A	997	AMP	C5-C4-N9	2.23	108.24	105.81
4	A	999	PLP	C6-C5-C4	2.20	119.90	118.10
5	A	913	AMP	C5-C6-N6	2.18	128.68	123.29
5	A	913	AMP	C5'-C4'-C3'	2.13	122.90	115.21
5	A	997	AMP	C2'-C3'-C4'	-2.09	98.56	102.61
5	A	997	AMP	C5-C6-N6	-2.09	118.10	123.29
5	A	913	AMP	O3'-C3'-C4'	2.06	117.00	111.08
5	A	997	AMP	C4-N9-C8	2.01	107.85	105.74

There are no chirality outliers.

All (5) torsion outliers are listed below:

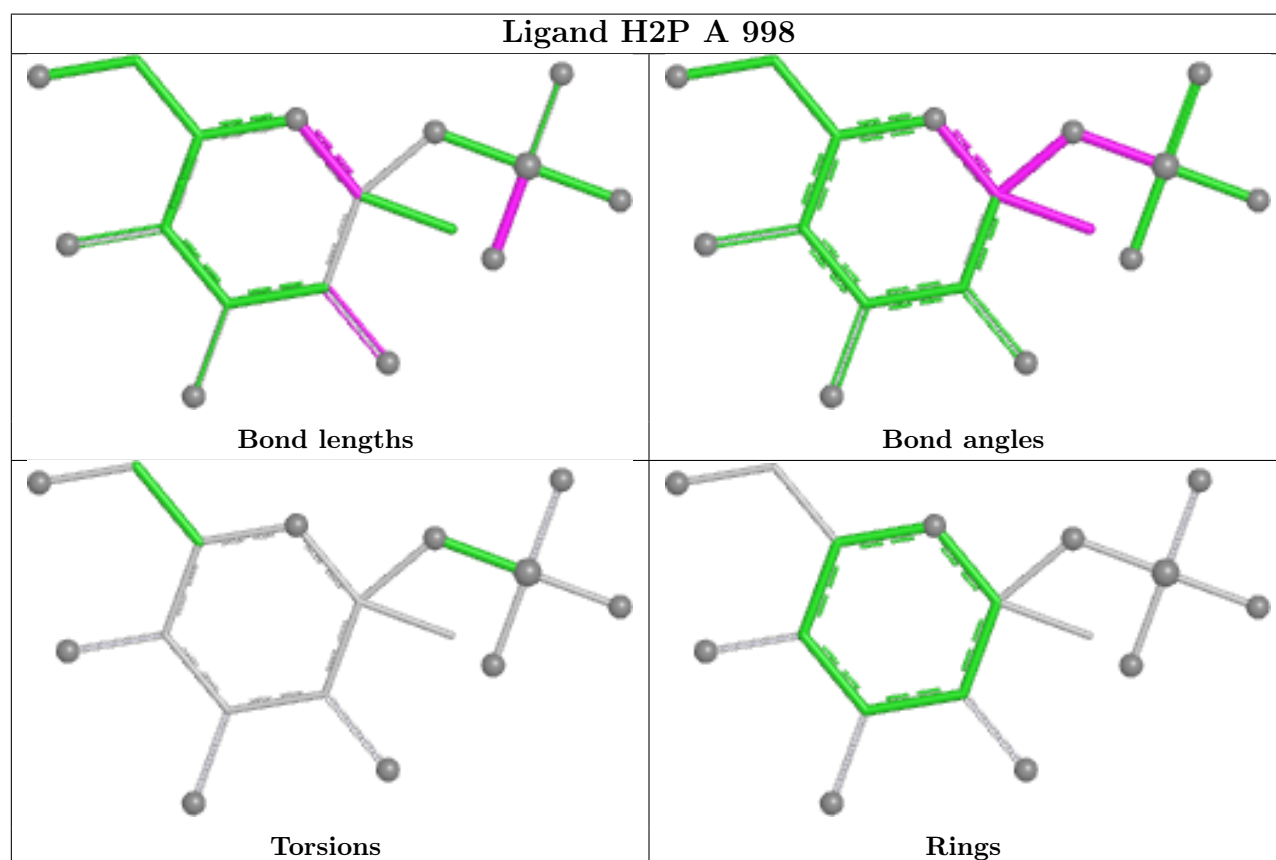
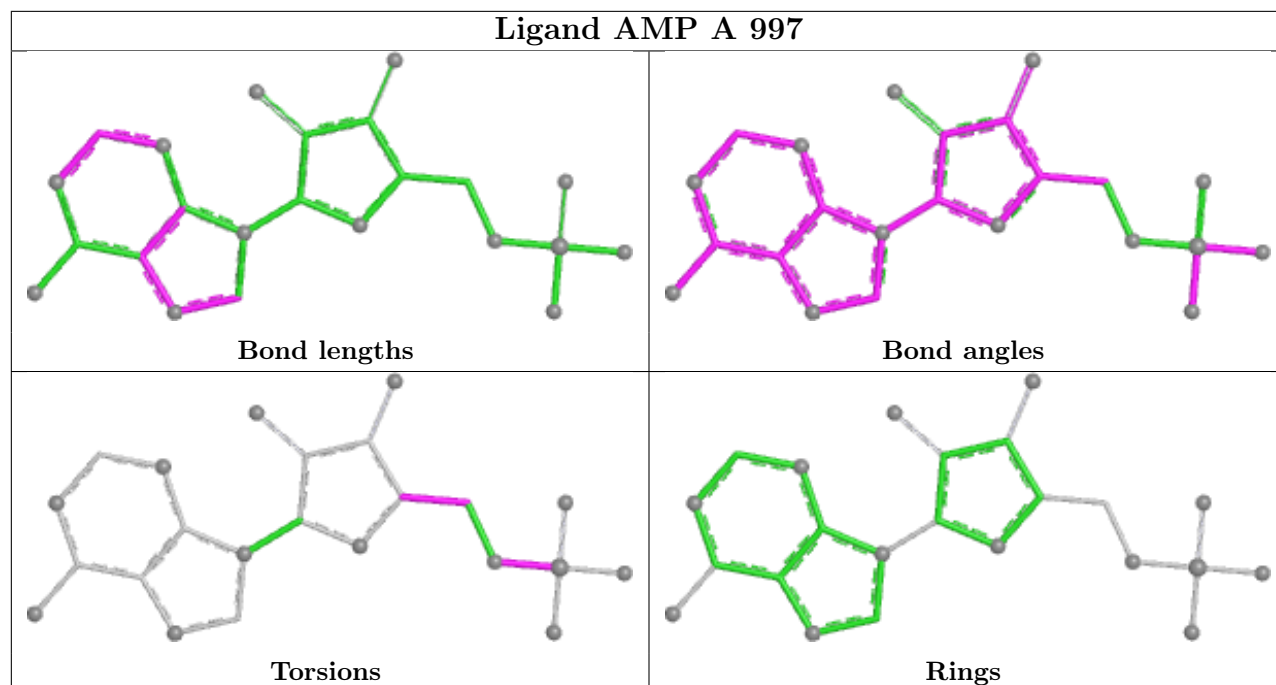
Mol	Chain	Res	Type	Atoms
5	A	913	AMP	C5'-O5'-P-O2P
5	A	913	AMP	C5'-O5'-P-O3P
5	A	997	AMP	C5'-O5'-P-O1P
5	A	997	AMP	O4'-C4'-C5'-O5'
5	A	913	AMP	C2'-C1'-N9-C4

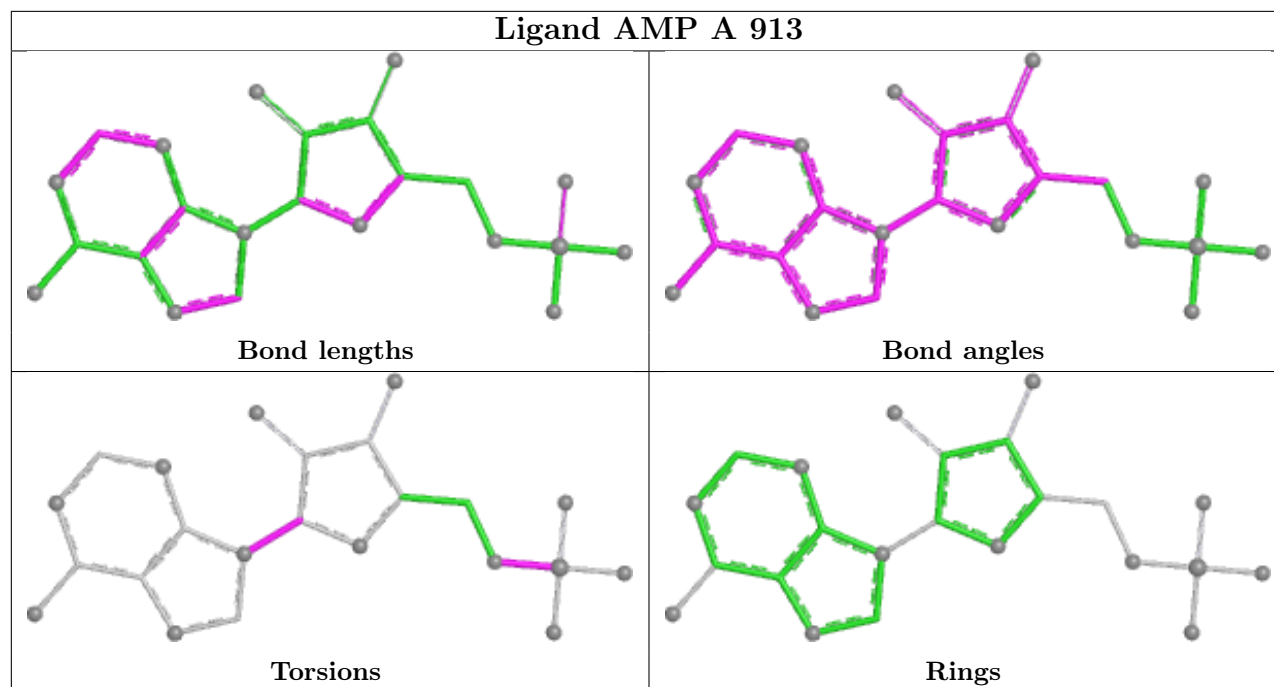
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	998	H2P	9	0
5	A	913	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	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	281:PRO	C	282:ASN	N	1.16
1	A	41:LYS	C	42:ASP	N	1.13
1	A	282:ASN	C	283:ASP	N	0.94

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.