



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:07 PM UTC

PDB ID : 5ABP / pdb_00005abp
Title : SUBSTRATE SPECIFICITY AND AFFINITY OF A PROTEIN MODULATED BY BOUND WATER MOLECULES
Authors : Quiocho, F.A.; Wilson, D.K.; Vyas, N.K.
Deposited on : 1990-12-26
Resolution : 1.80 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
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

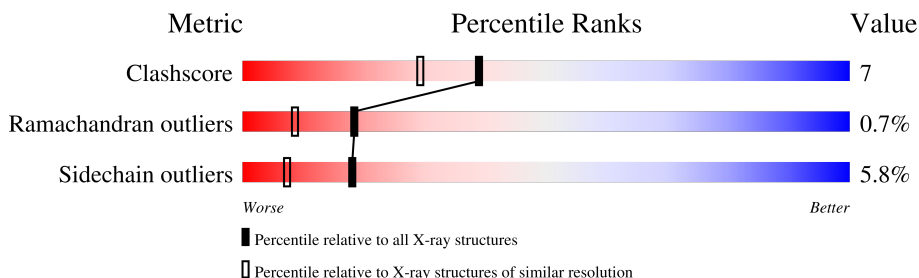
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	306	

2 Entry composition [i](#)

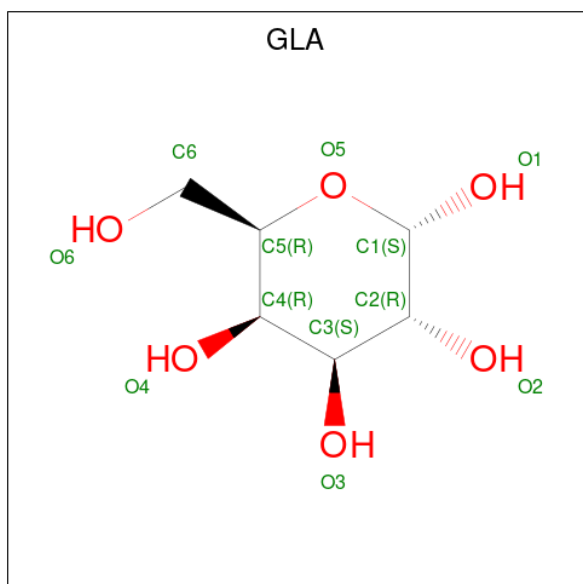
There are 4 unique types of molecules in this entry. The entry contains 2576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ARABINOSE-BINDING PROTEIN.

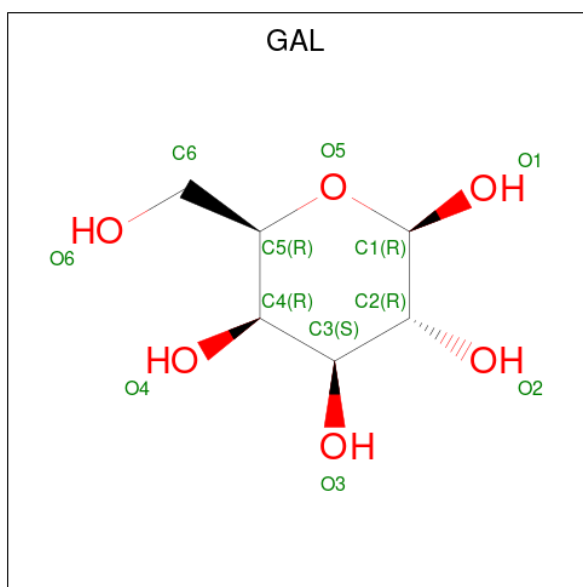
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2316	1473	389	443	11	0	0	0

- Molecule 2 is alpha-D-galactopyranose (CCD ID: GLA) (formula: $C_6H_{12}O_6$).



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

- Molecule 3 is beta-D-galactopyranose (CCD ID: GAL) (formula: $C_6H_{12}O_6$).



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

- Molecule 4 is water.

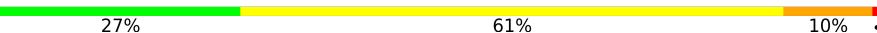
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	236	Total	O	0	0
			236	236		

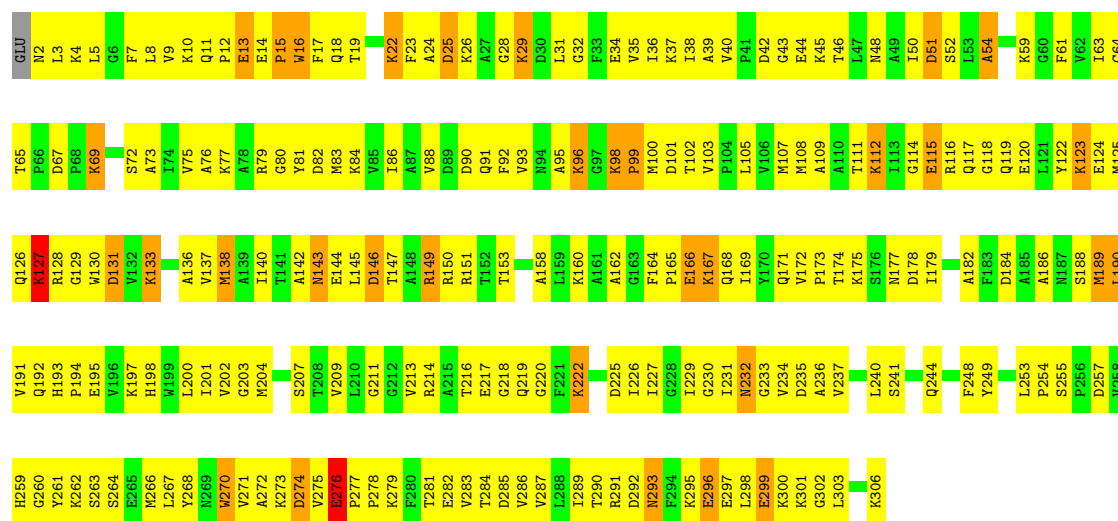
3 Residue-property plots

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: L-ARABINOSE-BINDING PROTEIN

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.92Å 72.02Å 78.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.132 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2576	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: GAL, GLA

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	2.66	161/2361 (6.8%)	3.01	289/3189 (9.1%)

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	LYS	N-CA	11.69	1.61	1.46
1	A	193	HIS	C-O	11.27	1.36	1.24
1	A	83	MET	N-CA	10.40	1.58	1.46
1	A	35	VAL	CA-CB	9.24	1.65	1.54
1	A	263	SER	N-CA	9.23	1.57	1.46
1	A	179	ILE	CA-CB	9.18	1.59	1.54
1	A	231	ILE	C-O	9.11	1.33	1.24
1	A	44	GLU	CA-CB	8.81	1.67	1.53
1	A	126	GLN	N-CA	8.73	1.56	1.46
1	A	125	MET	CA-C	8.69	1.64	1.52
1	A	248	PHE	CA-C	8.57	1.63	1.52
1	A	147	THR	CB-OG1	8.48	1.57	1.43
1	A	249	TYR	C-O	8.46	1.34	1.24
1	A	174	THR	CA-C	7.99	1.62	1.52
1	A	127	LYS	C-N	7.90	1.45	1.33
1	A	86	ILE	N-CA	7.84	1.55	1.46
1	A	75	VAL	CA-C	7.81	1.62	1.52
1	A	292	ASP	C-O	7.78	1.34	1.24
1	A	11	GLN	CA-CB	7.64	1.63	1.53
1	A	12	PRO	C-N	-7.60	1.22	1.33
1	A	109	ALA	C-O	7.58	1.32	1.23
1	A	291	ARG	C-O	-7.57	1.14	1.24
1	A	46	THR	CA-CB	7.49	1.65	1.53
1	A	67	ASP	N-CA	7.49	1.56	1.46
1	A	64	CYS	CA-C	7.47	1.62	1.53
1	A	126	GLN	C-O	7.37	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	PRO	CA-CB	7.36	1.62	1.53
1	A	147	THR	C-O	7.32	1.32	1.24
1	A	112	LYS	C-O	7.21	1.32	1.24
1	A	102	THR	CA-CB	7.20	1.66	1.53
1	A	77	LYS	CA-CB	-7.19	1.42	1.53
1	A	267	LEU	N-CA	7.16	1.54	1.46
1	A	9	VAL	C-O	7.14	1.31	1.24
1	A	92	PHE	N-CA	7.09	1.54	1.46
1	A	173	PRO	N-CD	7.08	1.57	1.47
1	A	38	ILE	N-CA	7.00	1.54	1.46
1	A	52	SER	C-O	6.99	1.32	1.24
1	A	105	LEU	CA-C	6.98	1.61	1.52
1	A	99	PRO	CA-CB	6.92	1.62	1.53
1	A	136	ALA	N-CA	6.88	1.54	1.46
1	A	261	TYR	CA-CB	6.86	1.64	1.53
1	A	153	THR	CA-CB	6.84	1.64	1.53
1	A	63	ILE	C-O	6.84	1.30	1.24
1	A	88	VAL	N-CA	6.75	1.53	1.46
1	A	5	LEU	N-CA	6.73	1.54	1.46
1	A	291	ARG	CZ-NH2	6.73	1.42	1.33
1	A	18	GLN	N-CA	6.72	1.54	1.46
1	A	165	PRO	C-N	-6.69	1.25	1.33
1	A	95	ALA	C-O	6.68	1.31	1.24
1	A	292	ASP	N-CA	6.66	1.54	1.46
1	A	293	ASN	N-CA	6.64	1.54	1.46
1	A	298	LEU	C-O	-6.59	1.15	1.24
1	A	128	ARG	NE-CZ	6.59	1.40	1.33
1	A	216	THR	CA-CB	6.51	1.63	1.53
1	A	100	MET	C-N	-6.50	1.24	1.33
1	A	34	GLU	CA-C	6.47	1.60	1.52
1	A	54	ALA	N-CA	6.41	1.54	1.46
1	A	86	ILE	C-N	-6.38	1.24	1.33
1	A	61	PHE	N-CA	6.27	1.53	1.45
1	A	17	PHE	N-CA	6.24	1.54	1.46
1	A	192	GLN	C-N	6.22	1.41	1.33
1	A	130	TRP	NE1-CE2	6.19	1.44	1.37
1	A	171	GLN	C-O	6.17	1.31	1.23
1	A	29	LYS	C-N	-6.15	1.26	1.33
1	A	19	THR	CB-OG1	6.12	1.53	1.43
1	A	36	ILE	CA-CB	6.12	1.61	1.54
1	A	98	LYS	CA-C	6.12	1.60	1.53
1	A	101	ASP	CA-CB	6.12	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ASP	C-N	6.09	1.42	1.33
1	A	236	ALA	N-CA	6.08	1.53	1.46
1	A	271	VAL	CA-CB	-6.01	1.47	1.54
1	A	202	VAL	CA-C	6.00	1.59	1.52
1	A	229	ILE	C-N	-6.00	1.24	1.33
1	A	115	GLU	N-CA	6.00	1.53	1.46
1	A	116	ARG	N-CA	5.98	1.53	1.46
1	A	108	MET	N-CA	5.98	1.53	1.45
1	A	81	TYR	N-CA	-5.98	1.39	1.46
1	A	203	GLY	N-CA	5.96	1.51	1.45
1	A	279	LYS	C-O	-5.96	1.16	1.24
1	A	218	GLY	N-CA	5.91	1.53	1.45
1	A	237	VAL	C-O	5.83	1.30	1.24
1	A	8	LEU	N-CA	5.80	1.53	1.46
1	A	39	ALA	C-O	5.80	1.30	1.24
1	A	16	TRP	C-O	5.78	1.30	1.24
1	A	289	ILE	C-O	5.77	1.30	1.24
1	A	186	ALA	C-O	-5.74	1.17	1.24
1	A	149	ARG	CZ-NH1	5.74	1.40	1.32
1	A	234	VAL	CA-CB	5.74	1.62	1.54
1	A	189	MET	CA-CB	-5.71	1.44	1.53
1	A	76	ALA	C-N	-5.70	1.26	1.33
1	A	214	ARG	NE-CZ	5.69	1.39	1.33
1	A	299	GLU	C-N	-5.68	1.26	1.34
1	A	253	LEU	CA-CB	5.68	1.62	1.52
1	A	69	LYS	C-O	5.68	1.31	1.24
1	A	284	THR	CA-CB	5.68	1.63	1.53
1	A	184	ASP	CG-OD2	5.67	1.36	1.25
1	A	201	ILE	CA-CB	5.63	1.60	1.54
1	A	12	PRO	N-CD	5.63	1.55	1.47
1	A	32	GLY	N-CA	-5.63	1.37	1.45
1	A	35	VAL	N-CA	5.61	1.53	1.46
1	A	36	ILE	C-O	5.61	1.30	1.24
1	A	222	LYS	N-CA	5.61	1.52	1.45
1	A	219	GLN	C-O	-5.58	1.16	1.24
1	A	178	ASP	C-O	-5.57	1.17	1.23
1	A	293	ASN	CA-C	-5.56	1.45	1.52
1	A	138	MET	CA-CB	-5.50	1.46	1.53
1	A	69	LYS	N-CA	5.49	1.53	1.46
1	A	137	VAL	C-O	5.48	1.30	1.24
1	A	216	THR	CB-OG1	5.48	1.52	1.43
1	A	233	GLY	C-N	5.48	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	HIS	N-CA	5.45	1.52	1.46
1	A	10	LYS	C-O	5.44	1.30	1.24
1	A	118	GLY	CA-C	5.44	1.58	1.52
1	A	131	ASP	N-CA	5.42	1.52	1.46
1	A	72	SER	N-CA	5.41	1.52	1.46
1	A	129	GLY	N-CA	-5.41	1.38	1.45
1	A	10	LYS	CA-C	-5.41	1.45	1.52
1	A	64	CYS	C-O	-5.41	1.17	1.24
1	A	13	GLU	CD-OE1	-5.41	1.15	1.25
1	A	103	VAL	CA-C	5.40	1.58	1.52
1	A	15	PRO	CA-CB	5.39	1.61	1.53
1	A	93	VAL	CA-C	5.38	1.59	1.52
1	A	138	MET	N-CA	5.38	1.52	1.46
1	A	88	VAL	C-O	5.37	1.29	1.24
1	A	130	TRP	CA-CB	5.37	1.62	1.53
1	A	140	ILE	N-CA	5.36	1.52	1.46
1	A	46	THR	CA-C	-5.35	1.46	1.52
1	A	193	HIS	C-N	-5.33	1.27	1.34
1	A	190	LEU	CB-CG	5.33	1.64	1.53
1	A	120	GLU	C-O	5.32	1.30	1.24
1	A	7	PHE	C-N	5.32	1.40	1.33
1	A	194	PRO	N-CD	5.29	1.55	1.47
1	A	131	ASP	C-N	-5.28	1.27	1.34
1	A	144	GLU	C-O	5.27	1.30	1.24
1	A	5	LEU	C-O	5.26	1.30	1.23
1	A	168	GLN	N-CA	5.25	1.52	1.46
1	A	277	PRO	CA-C	-5.23	1.47	1.52
1	A	13	GLU	CD-OE2	5.23	1.35	1.25
1	A	76	ALA	N-CA	5.23	1.52	1.46
1	A	248	PHE	C-N	-5.20	1.26	1.33
1	A	291	ARG	CA-C	5.20	1.59	1.52
1	A	77	LYS	C-N	5.18	1.40	1.33
1	A	10	LYS	C-N	5.17	1.40	1.33
1	A	42	ASP	N-CA	5.17	1.52	1.45
1	A	195	GLU	CG-CD	-5.17	1.39	1.52
1	A	137	VAL	CA-C	-5.16	1.46	1.52
1	A	171	GLN	C-N	-5.15	1.27	1.33
1	A	114	GLY	C-O	5.14	1.29	1.23
1	A	65	THR	CA-C	-5.14	1.47	1.53
1	A	91	GLN	C-N	-5.12	1.26	1.33
1	A	19	THR	CA-C	-5.11	1.46	1.52
1	A	169	ILE	C-O	5.10	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ALA	C-N	5.09	1.40	1.33
1	A	278	PRO	C-N	-5.06	1.26	1.34
1	A	219	GLN	CA-CB	5.05	1.61	1.53
1	A	162	ALA	CA-CB	-5.04	1.44	1.53
1	A	88	VAL	CA-CB	-5.02	1.47	1.55
1	A	302	GLY	CA-C	-5.02	1.44	1.51
1	A	230	GLY	C-O	5.02	1.29	1.23
1	A	182	ALA	CA-C	-5.01	1.45	1.52
1	A	198	HIS	CG-ND1	5.01	1.43	1.38

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NE-CZ-NH1	20.79	142.29	121.50
1	A	79	ARG	CD-NE-CZ	19.51	151.71	124.40
1	A	101	ASP	CA-CB-CG	-13.93	98.67	112.60
1	A	123	LYS	CA-CB-CG	13.10	140.30	114.10
1	A	237	VAL	CA-C-O	-11.90	108.58	120.95
1	A	79	ARG	NH1-CZ-NH2	-11.70	104.09	119.30
1	A	167	LYS	CA-C-N	-11.43	105.37	122.86
1	A	167	LYS	C-N-CA	-11.43	105.37	122.86
1	A	268	TYR	CA-C-O	-11.43	108.82	120.82
1	A	67	ASP	CA-CB-CG	-11.22	101.38	112.60
1	A	249	TYR	O-C-N	-11.13	107.42	122.33
1	A	5	LEU	CA-C-O	-10.92	108.11	120.66
1	A	99	PRO	CA-C-O	-10.83	108.99	121.34
1	A	291	ARG	NE-CZ-NH1	10.48	131.98	121.50
1	A	119	GLN	OE1-CD-NE2	-10.44	112.16	122.60
1	A	193	HIS	CA-CB-CG	-10.29	103.51	113.80
1	A	143	ASN	OD1-CG-ND2	-10.13	112.47	122.60
1	A	145	LEU	CA-C-O	9.99	131.31	120.32
1	A	150	ARG	NE-CZ-NH2	-9.96	110.23	119.20
1	A	149	ARG	NE-CZ-NH2	-9.74	110.44	119.20
1	A	54	ALA	N-CA-CB	-9.72	95.84	110.12
1	A	150	ARG	CA-CB-CG	-9.51	95.09	114.10
1	A	211	GLY	O-C-N	-9.09	113.35	122.17
1	A	296	GLU	CB-CG-CD	-9.09	97.15	112.60
1	A	145	LEU	O-C-N	-9.08	112.55	123.27
1	A	79	ARG	CA-CB-CG	8.90	131.90	114.10
1	A	302	GLY	O-C-N	-8.78	111.28	122.43
1	A	270	TRP	CA-C-O	-8.69	110.60	120.24
1	A	191	VAL	CA-C-O	-8.56	108.32	119.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	CG-CD-NE	8.51	130.73	112.00
1	A	178	ASP	O-C-N	8.51	132.09	122.99
1	A	102	THR	OG1-CB-CG2	8.46	126.23	109.30
1	A	122	TYR	CA-C-O	-8.26	110.47	119.97
1	A	124	GLU	O-C-N	-8.23	112.77	122.15
1	A	182	ALA	O-C-N	-8.18	112.65	122.22
1	A	178	ASP	CA-C-N	-8.18	113.79	120.33
1	A	178	ASP	C-N-CA	-8.18	113.79	120.33
1	A	297	GLU	CA-C-O	-8.11	111.95	120.55
1	A	45	LYS	O-C-N	-8.10	112.75	122.22
1	A	130	TRP	CB-CG-CD2	-8.09	115.47	126.80
1	A	82	ASP	CA-CB-CG	-8.03	104.57	112.60
1	A	22	LYS	CA-CB-CG	7.93	129.97	114.10
1	A	281	THR	CA-C-O	7.93	128.64	120.24
1	A	93	VAL	CA-C-O	-7.92	113.35	121.67
1	A	150	ARG	NH1-CZ-NH2	7.83	129.49	119.30
1	A	278	PRO	CA-C-O	-7.82	112.48	121.56
1	A	18	GLN	OE1-CD-NE2	-7.78	114.83	122.60
1	A	75	VAL	O-C-N	7.72	129.78	121.83
1	A	200	LEU	CA-C-O	-7.69	112.05	120.43
1	A	274	ASP	CA-C-O	7.66	131.46	120.51
1	A	232	ASN	O-C-N	7.64	132.76	122.59
1	A	29	LYS	CB-CA-C	-7.63	98.90	110.88
1	A	147	THR	CA-CB-OG1	-7.61	98.18	109.60
1	A	24	ALA	N-CA-C	-7.60	103.08	111.36
1	A	126	GLN	CA-C-O	-7.55	112.89	120.82
1	A	191	VAL	O-C-N	7.53	132.54	122.31
1	A	244	GLN	N-CA-C	7.53	122.09	110.20
1	A	44	GLU	CA-CB-CG	-7.47	99.16	114.10
1	A	220	GLY	CA-C-O	-7.45	109.75	119.44
1	A	4	LYS	CA-CB-CG	-7.45	99.20	114.10
1	A	77	LYS	CG-CD-CE	-7.44	94.18	111.30
1	A	291	ARG	O-C-N	7.44	132.40	122.43
1	A	214	ARG	NE-CZ-NH2	7.40	125.86	119.20
1	A	82	ASP	N-CA-CB	7.40	123.30	112.13
1	A	79	ARG	CB-CG-CD	7.39	128.29	111.30
1	A	240	LEU	CA-C-O	-7.36	110.33	119.38
1	A	146	ASP	O-C-N	7.31	129.87	122.12
1	A	147	THR	CA-C-O	-7.29	112.82	120.55
1	A	130	TRP	CB-CG-CD1	7.27	137.81	126.90
1	A	232	ASN	CA-C-O	-7.25	110.14	120.51
1	A	167	LYS	O-C-N	7.16	132.99	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	MET	CA-C-N	7.12	135.14	121.54
1	A	100	MET	C-N-CA	7.12	135.14	121.54
1	A	77	LYS	CA-CB-CG	7.12	128.34	114.10
1	A	262	LYS	CA-CB-CG	-7.12	99.87	114.10
1	A	213	VAL	CA-C-O	-7.10	113.64	121.17
1	A	79	ARG	CA-C-N	7.07	127.94	120.03
1	A	79	ARG	C-N-CA	7.07	127.94	120.03
1	A	109	ALA	CA-C-N	7.05	130.06	120.54
1	A	109	ALA	C-N-CA	7.05	130.06	120.54
1	A	39	ALA	CA-C-O	-7.04	112.67	120.69
1	A	45	LYS	CA-C-O	7.01	128.02	120.10
1	A	13	GLU	CB-CG-CD	6.97	124.45	112.60
1	A	201	ILE	CA-C-N	6.94	131.68	122.93
1	A	201	ILE	C-N-CA	6.94	131.68	122.93
1	A	96	LYS	CG-CD-CE	6.92	127.23	111.30
1	A	124	GLU	OE1-CD-OE2	6.91	139.49	122.90
1	A	105	LEU	O-C-N	6.91	131.70	123.27
1	A	300	LYS	CA-CB-CG	6.88	127.86	114.10
1	A	12	PRO	N-CD-CG	-6.86	92.91	103.20
1	A	31	LEU	O-C-N	-6.86	112.67	122.41
1	A	43	GLY	O-C-N	-6.86	114.93	122.68
1	A	76	ALA	N-CA-C	-6.81	103.78	111.07
1	A	165	PRO	CA-C-O	-6.81	114.12	121.27
1	A	50	ILE	CA-C-N	-6.80	111.16	120.28
1	A	50	ILE	C-N-CA	-6.80	111.16	120.28
1	A	271	VAL	CA-C-N	6.79	132.23	120.68
1	A	271	VAL	C-N-CA	6.79	132.23	120.68
1	A	182	ALA	CA-C-O	6.78	127.76	120.10
1	A	119	GLN	CG-CD-OE1	6.77	134.35	120.80
1	A	117	GLN	OE1-CD-NE2	6.77	129.37	122.60
1	A	76	ALA	O-C-N	-6.73	115.14	122.07
1	A	131	ASP	CA-C-O	-6.73	113.02	120.69
1	A	168	GLN	N-CA-C	-6.71	103.40	112.26
1	A	287	VAL	CG1-CB-CG2	-6.69	96.09	110.80
1	A	209	VAL	CB-CA-C	6.66	120.74	112.02
1	A	79	ARG	N-CA-C	-6.66	104.02	111.28
1	A	25	ASP	CA-CB-CG	-6.64	105.95	112.60
1	A	103	VAL	O-C-N	6.64	128.67	121.10
1	A	303	LEU	CB-CA-C	6.58	119.31	111.22
1	A	227	ILE	CA-C-O	-6.57	113.63	120.27
1	A	93	VAL	O-C-N	6.49	130.25	123.04
1	A	167	LYS	CA-C-O	-6.47	110.64	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	PHE	O-C-N	6.46	130.89	122.68
1	A	296	GLU	OE1-CD-OE2	6.45	138.39	122.90
1	A	260	GLY	O-C-N	-6.45	115.99	122.18
1	A	271	VAL	O-C-N	-6.44	115.20	121.90
1	A	14	GLU	CB-CA-C	-6.43	99.81	109.26
1	A	272	ALA	CA-C-N	6.43	133.04	121.15
1	A	272	ALA	C-N-CA	6.43	133.04	121.15
1	A	219	GLN	CG-CD-NE2	6.42	126.03	116.40
1	A	122	TYR	O-C-N	6.41	130.16	122.27
1	A	37	LYS	CG-CD-CE	6.41	126.04	111.30
1	A	274	ASP	O-C-N	-6.40	114.08	122.59
1	A	263	SER	CA-C-N	6.39	129.36	120.29
1	A	263	SER	C-N-CA	6.39	129.36	120.29
1	A	69	LYS	CA-CB-CG	-6.35	101.40	114.10
1	A	300	LYS	CB-CA-C	-6.33	98.92	110.63
1	A	286	VAL	CA-C-O	-6.32	112.88	120.78
1	A	117	GLN	CA-C-N	6.27	126.94	119.98
1	A	117	GLN	C-N-CA	6.27	126.94	119.98
1	A	301	LYS	N-CA-C	-6.25	105.24	112.92
1	A	211	GLY	CA-C-N	6.25	133.65	121.41
1	A	211	GLY	C-N-CA	6.25	133.65	121.41
1	A	36	ILE	CA-C-O	-6.23	113.36	120.65
1	A	79	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	A	235	ASP	CB-CG-OD1	6.22	132.70	118.40
1	A	42	ASP	N-CA-C	-6.18	99.75	108.96
1	A	291	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	A	193	HIS	CA-C-N	6.17	125.79	119.56
1	A	193	HIS	C-N-CA	6.17	125.79	119.56
1	A	248	PHE	CA-C-O	-6.16	114.51	120.92
1	A	299	GLU	N-CA-C	-6.15	104.66	111.36
1	A	115	GLU	OE1-CD-OE2	6.09	137.52	122.90
1	A	128	ARG	CA-C-N	6.08	131.76	120.87
1	A	128	ARG	C-N-CA	6.08	131.76	120.87
1	A	38	ILE	CA-C-N	6.08	130.19	121.50
1	A	38	ILE	C-N-CA	6.08	130.19	121.50
1	A	291	ARG	CA-C-O	-6.07	111.91	119.38
1	A	28	GLY	N-CA-C	-6.07	105.45	112.73
1	A	216	THR	OG1-CB-CG2	6.05	121.41	109.30
1	A	276	GLU	CB-CA-C	-6.04	99.79	109.69
1	A	90	ASP	N-CA-CB	-6.03	101.11	110.57
1	A	222	LYS	N-CA-C	-6.01	101.88	110.59
1	A	219	GLN	N-CA-CB	6.01	118.85	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ALA	N-CA-CB	-5.99	101.81	110.56
1	A	179	ILE	O-C-N	-5.99	116.59	120.42
1	A	98	LYS	CA-CB-CG	5.98	126.06	114.10
1	A	99	PRO	N-CA-CB	-5.98	97.99	103.31
1	A	130	TRP	N-CA-CB	-5.97	101.26	110.04
1	A	293	ASN	CB-CG-ND2	5.95	125.33	116.40
1	A	192	GLN	CB-CG-CD	-5.95	102.48	112.60
1	A	296	GLU	CG-CD-OE2	-5.93	104.75	118.40
1	A	116	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	A	125	MET	CA-CB-CG	-5.90	102.30	114.10
1	A	276	GLU	OE1-CD-OE2	5.90	137.06	122.90
1	A	151	ARG	O-C-N	-5.89	115.73	122.09
1	A	142	ALA	N-CA-C	-5.88	98.78	108.49
1	A	241	SER	CA-CB-OG	-5.88	99.34	111.10
1	A	102	THR	N-CA-C	5.86	120.58	113.38
1	A	301	LYS	CB-CG-CD	5.84	124.73	111.30
1	A	270	TRP	N-CA-C	-5.77	104.59	111.69
1	A	76	ALA	CA-C-N	5.76	127.93	120.44
1	A	76	ALA	C-N-CA	5.76	127.93	120.44
1	A	192	GLN	CA-C-N	-5.76	115.91	123.34
1	A	192	GLN	C-N-CA	-5.76	115.91	123.34
1	A	197	LYS	CB-CG-CD	5.75	124.52	111.30
1	A	153	THR	CA-C-N	5.73	126.45	120.03
1	A	153	THR	C-N-CA	5.73	126.45	120.03
1	A	54	ALA	CA-C-O	-5.73	114.48	120.55
1	A	249	TYR	N-CA-CB	-5.72	101.49	110.30
1	A	22	LYS	CB-CG-CD	-5.72	98.14	111.30
1	A	249	TYR	CA-CB-CG	-5.70	103.63	113.90
1	A	111	THR	O-C-N	5.69	127.93	122.07
1	A	105	LEU	CA-C-O	-5.69	114.12	120.66
1	A	28	GLY	CA-C-O	-5.68	114.90	120.75
1	A	34	GLU	N-CA-CB	-5.68	101.55	110.69
1	A	211	GLY	CA-C-O	5.67	126.36	120.80
1	A	153	THR	CA-C-O	-5.66	114.87	120.82
1	A	296	GLU	CB-CA-C	-5.66	101.99	110.88
1	A	18	GLN	CA-CB-CG	-5.66	102.79	114.10
1	A	244	GLN	OE1-CD-NE2	5.66	128.26	122.60
1	A	116	ARG	O-C-N	-5.65	116.13	122.12
1	A	102	THR	CA-CB-OG1	-5.64	101.13	109.60
1	A	109	ALA	N-CA-CB	-5.63	102.47	110.58
1	A	255	SER	CA-CB-OG	-5.62	99.86	111.10
1	A	77	LYS	N-CA-CB	5.62	118.16	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ASP	O-C-N	5.61	129.92	122.41
1	A	175	LYS	CA-CB-CG	-5.60	102.91	114.10
1	A	171	GLN	CB-CG-CD	-5.59	103.09	112.60
1	A	111	THR	CA-CB-OG1	-5.59	101.22	109.60
1	A	144	GLU	CB-CG-CD	5.58	122.09	112.60
1	A	281	THR	O-C-N	-5.58	116.74	123.27
1	A	91	GLN	O-C-N	5.58	129.59	123.01
1	A	76	ALA	CA-C-O	-5.55	114.99	120.82
1	A	22	LYS	CB-CA-C	-5.54	101.59	110.79
1	A	51	ASP	CA-C-N	5.54	127.70	120.28
1	A	51	ASP	C-N-CA	5.54	127.70	120.28
1	A	34	GLU	CB-CG-CD	-5.54	103.19	112.60
1	A	51	ASP	CA-CB-CG	-5.52	107.08	112.60
1	A	65	THR	CA-CB-OG1	-5.50	101.35	109.60
1	A	166	GLU	O-C-N	-5.50	116.30	122.12
1	A	117	GLN	O-C-N	-5.49	116.41	122.07
1	A	283	VAL	N-CA-CB	-5.49	104.79	111.21
1	A	272	ALA	N-CA-C	5.46	119.11	112.23
1	A	13	GLU	CG-CD-OE1	5.46	130.97	118.40
1	A	67	ASP	N-CA-CB	-5.46	100.66	110.37
1	A	13	GLU	CG-CD-OE2	-5.44	105.88	118.40
1	A	190	LEU	O-C-N	5.43	127.67	122.07
1	A	209	VAL	N-CA-C	-5.42	105.43	110.53
1	A	120	GLU	OE1-CD-OE2	5.42	135.90	122.90
1	A	67	ASP	CB-CG-OD2	-5.41	105.95	118.40
1	A	93	VAL	CA-C-N	-5.41	112.94	121.86
1	A	93	VAL	C-N-CA	-5.41	112.94	121.86
1	A	207	SER	CA-CB-OG	-5.40	100.29	111.10
1	A	201	ILE	CA-CB-CG1	-5.40	101.23	110.40
1	A	292	ASP	CB-CG-OD2	-5.40	105.99	118.40
1	A	292	ASP	CA-C-N	-5.39	113.50	122.08
1	A	292	ASP	C-N-CA	-5.39	113.50	122.08
1	A	40	VAL	CA-CB-CG2	5.38	119.55	110.40
1	A	193	HIS	ND1-CG-CD2	5.38	111.47	106.10
1	A	225	ASP	CA-CB-CG	-5.36	107.24	112.60
1	A	267	LEU	CA-C-O	5.36	126.45	120.82
1	A	296	GLU	N-CA-CB	5.35	117.77	110.01
1	A	271	VAL	CA-CB-CG1	5.35	119.49	110.40
1	A	282	GLU	CG-CD-OE1	-5.34	106.11	118.40
1	A	149	ARG	N-CA-C	5.33	117.78	111.33
1	A	80	GLY	O-C-N	-5.32	117.01	122.17
1	A	107	MET	O-C-N	5.30	129.20	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	GLY	CA-C-O	5.30	125.00	119.06
1	A	217	GLU	CA-C-O	5.30	126.16	120.55
1	A	232	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	A	226	ILE	CA-C-N	-5.29	115.46	122.98
1	A	226	ILE	C-N-CA	-5.29	115.46	122.98
1	A	116	ARG	CD-NE-CZ	-5.28	117.01	124.40
1	A	158	ALA	O-C-N	5.28	128.16	122.15
1	A	23	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	248	PHE	N-CA-C	-5.27	98.72	107.99
1	A	278	PRO	N-CA-C	-5.25	102.86	111.21
1	A	11	GLN	CA-CB-CG	-5.24	103.61	114.10
1	A	138	MET	N-CA-C	-5.24	100.18	108.73
1	A	203	GLY	O-C-N	-5.22	118.70	123.56
1	A	209	VAL	CA-C-O	-5.21	115.26	121.05
1	A	287	VAL	CA-CB-CG1	5.18	119.21	110.40
1	A	48	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	234	VAL	CA-C-O	-5.18	114.88	120.47
1	A	138	MET	CB-CG-SD	-5.16	97.21	112.70
1	A	118	GLY	O-C-N	5.16	127.15	122.19
1	A	29	LYS	O-C-N	-5.15	116.76	122.07
1	A	253	LEU	N-CA-CB	-5.15	103.63	110.17
1	A	131	ASP	O-C-N	5.12	129.04	123.04
1	A	10	LYS	N-CA-CB	-5.11	102.36	110.28
1	A	149	ARG	NH1-CZ-NH2	5.11	125.94	119.30
1	A	290	THR	CA-CB-CG2	5.11	119.19	110.50
1	A	237	VAL	N-CA-C	-5.10	105.42	110.62
1	A	219	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	257	ASP	N-CA-C	-5.10	105.72	111.28
1	A	143	ASN	N-CA-CB	-5.10	101.47	110.39
1	A	195	GLU	CA-C-N	-5.09	115.80	122.37
1	A	195	GLU	C-N-CA	-5.09	115.80	122.37
1	A	4	LYS	O-C-N	5.08	129.16	123.27
1	A	166	GLU	CA-C-O	5.08	126.12	120.63
1	A	130	TRP	O-C-N	-5.07	116.57	122.81
1	A	162	ALA	CA-C-N	-5.07	113.93	122.25
1	A	162	ALA	C-N-CA	-5.07	113.93	122.25
1	A	35	VAL	CA-C-O	-5.07	115.11	120.53
1	A	177	ASN	CA-C-O	-5.07	114.83	122.38
1	A	4	LYS	CA-C-N	-5.06	114.53	122.73
1	A	4	LYS	C-N-CA	-5.06	114.53	122.73
1	A	279	LYS	CB-CA-C	-5.05	100.98	110.67
1	A	2	ASN	CA-C-N	5.05	128.27	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ASN	C-N-CA	5.05	128.27	121.05
1	A	164	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	264	SER	CA-C-O	-5.04	115.08	120.42
1	A	292	ASP	CA-C-O	-5.04	113.85	119.79
1	A	188	SER	CB-CA-C	5.03	119.40	110.85
1	A	119	GLN	CA-C-O	-5.02	115.10	120.42
1	A	201	ILE	N-CA-CB	-5.01	105.14	111.46
1	A	268	TYR	CD1-CG-CD2	5.00	125.61	118.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2316	0	2326	32	0
2	A	12	0	12	0	0
3	A	12	0	11	1	0
4	A	236	0	0	11	1
All	All	2576	0	2349	32	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 7.

All (32) 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:146:ASP:HB2	4:A:503:HOH:O	1.45	1.16
1:A:276:GLU:HA	1:A:276:GLU:OE1	1.65	0.92
1:A:115:GLU:OE1	4:A:493:HOH:O	1.95	0.85
1:A:295:LYS:HD2	4:A:518:HOH:O	1.79	0.80
1:A:276:GLU:OE1	1:A:276:GLU:CA	2.30	0.79
1:A:296:GLU:HG3	4:A:341:HOH:O	1.81	0.79
1:A:296:GLU:CD	4:A:416:HOH:O	2.29	0.75
1:A:69:LYS:NZ	4:A:490:HOH:O	1.80	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:CB	4:A:503:HOH:O	2.18	0.71
1:A:160:LYS:HD3	1:A:166:GLU:HG2	1.78	0.64
1:A:273:LYS:O	1:A:274:ASP:C	2.41	0.64
1:A:295:LYS:HE3	1:A:306:LYS:O	1.98	0.63
1:A:26:LYS:HA	1:A:29:LYS:HD2	1.81	0.63
1:A:306:LYS:C	4:A:494:HOH:O	2.41	0.62
1:A:273:LYS:O	1:A:275:VAL:HG23	2.00	0.61
1:A:84:LYS:HD2	1:A:270:TRP:CE2	2.36	0.60
1:A:143:ASN:OD1	1:A:149:ARG:HG3	2.00	0.60
1:A:273:LYS:HB2	1:A:275:VAL:HG23	1.84	0.60
1:A:295:LYS:CE	1:A:306:LYS:O	2.51	0.59
1:A:69:LYS:CE	4:A:490:HOH:O	2.42	0.54
1:A:138:MET:HE1	1:A:190:LEU:HG	1.91	0.53
1:A:131:ASP:OD1	1:A:133:LYS:HG3	2.09	0.52
1:A:123:LYS:O	1:A:127:LYS:NZ	2.46	0.47
1:A:172:VAL:HB	1:A:189:MET:HE3	1.97	0.46
1:A:146:ASP:CG	4:A:503:HOH:O	2.50	0.45
1:A:293:ASN:OD1	1:A:293:ASN:C	2.57	0.45
1:A:16:TRP:CZ2	3:A:308[B]:GAL:H62	2.52	0.45
1:A:51:ASP:O	1:A:54:ALA:HB3	2.16	0.45
1:A:112:LYS:HA	1:A:112:LYS:HD3	1.58	0.44
1:A:222:LYS:NZ	4:A:444:HOH:O	2.52	0.43
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.85	0.41
1:A:25:ASP:O	1:A:29:LYS:HG3	2.21	0.41

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)
4:A:378:HOH:O	4:A:535:HOH:O[4_466]	1.82	0.38

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	303/306 (99%)	293 (97%)	8 (3%)	2 (1%)	18 8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	254	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	243/246 (99%)	229 (94%)	14 (6%)	18 7

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	15	PRO
1	A	22	LYS
1	A	59	LYS
1	A	96	LYS
1	A	98	LYS
1	A	99	PRO
1	A	127	LYS
1	A	133	LYS
1	A	167	LYS
1	A	204	MET
1	A	266	MET
1	A	276	GLU
1	A	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GAL	A	308[B]	-	12,12,12	1.81	2 (16%)	17,17,17	1.61	2 (11%)
2	GLA	A	307[A]	-	12,12,12	1.40	2 (16%)	17,17,17	1.52	4 (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
3	GAL	A	308[B]	-	-	0/2/22/22	0/1/1/1
2	GLA	A	307[A]	-	-	0/2/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	308[B]	GAL	C3-C2	-5.17	1.38	1.52
3	A	308[B]	GAL	C4-C3	2.64	1.59	1.52
2	A	307[A]	GLA	O2-C2	2.53	1.49	1.43
2	A	307[A]	GLA	O5-C1	2.03	1.47	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	308[B]	GAL	O3-C3-C2	4.05	119.92	110.38
2	A	307[A]	GLA	O4-C4-C5	2.84	116.32	109.32
2	A	307[A]	GLA	O5-C5-C6	-2.33	100.67	106.44
3	A	308[B]	GAL	O4-C4-C5	2.11	114.52	109.32
2	A	307[A]	GLA	C1-O5-C5	-2.11	109.57	113.65
2	A	307[A]	GLA	O6-C6-C5	-2.10	104.19	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	308[B]	GAL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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.