



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:20 PM GMT

PDB ID : 5ABP
Title : SUBSTRATE SPECIFICITY AND AFFINITY OF A PROTEIN MODU-
LATED 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

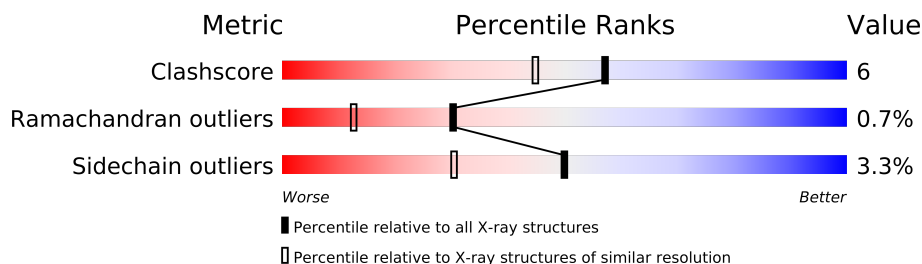
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	

2 Entry composition i

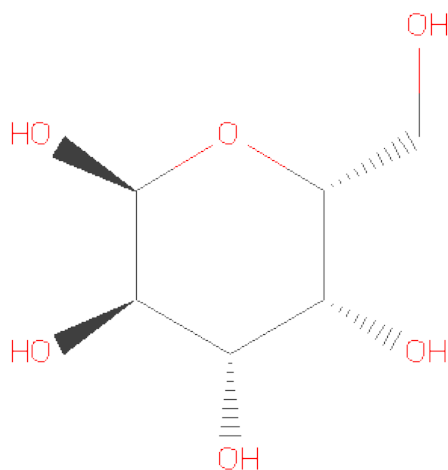
There are 4 unique types of molecules in this entry. The entry contains 2576 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

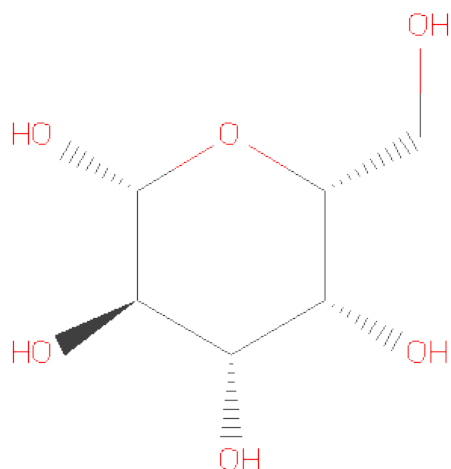
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2316	1473	389	443	11	0	0	0

- Molecule 2 is SUGAR (2-MER) (three-letter code: GLA) (formula: C₆H₁₂O₆).



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

- Molecule 3 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C₆H₁₂O₆).



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

- Molecule 4 is water.

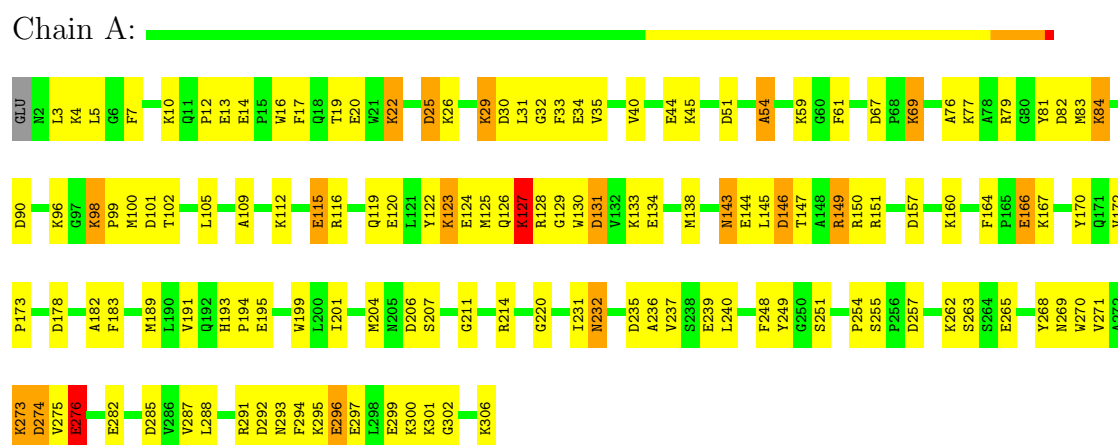
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	236	Total	O	0	0
			236	236		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: L-ARABINOSE-BINDING PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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: GLA, GAL

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	2.05	50/2361 (2.1%)	2.75	162/3189 (5.1%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	GLU	CD-OE1	-9.61	1.15	1.25
1	A	13	GLU	CD-OE2	8.76	1.35	1.25
1	A	195	GLU	CG-CD	-8.54	1.39	1.51
1	A	120	GLU	CD-OE1	-8.29	1.16	1.25
1	A	10	LYS	N-CA	7.46	1.61	1.46
1	A	147	THR	CB-OG1	7.04	1.57	1.43
1	A	291	ARG	CZ-NH2	7.04	1.42	1.33
1	A	173	PRO	N-CD	7.01	1.57	1.47
1	A	265	GLU	CD-OE2	-6.97	1.18	1.25
1	A	193	HIS	C-O	6.92	1.36	1.23
1	A	144	GLU	CD-OE2	6.73	1.33	1.25
1	A	251	SER	CB-OG	6.66	1.50	1.42
1	A	83	MET	N-CA	6.16	1.58	1.46
1	A	249	TYR	C-O	6.12	1.34	1.23
1	A	120	GLU	CD-OE2	-6.07	1.19	1.25
1	A	44	GLU	CA-CB	6.06	1.67	1.53
1	A	84	LYS	CD-CE	5.98	1.66	1.51
1	A	124	GLU	CD-OE2	-5.95	1.19	1.25
1	A	149	ARG	CZ-NH1	5.95	1.40	1.33
1	A	20	GLU	CD-OE2	-5.93	1.19	1.25
1	A	33	PHE	CG-CD2	5.91	1.47	1.38
1	A	32	GLY	N-CA	-5.89	1.37	1.46
1	A	296	GLU	CD-OE2	5.84	1.32	1.25
1	A	124	GLU	CG-CD	5.78	1.60	1.51
1	A	255	SER	CB-OG	5.68	1.49	1.42
1	A	292	ASP	C-O	5.66	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	SER	CA-CB	5.59	1.61	1.52
1	A	263	SER	N-CA	5.59	1.57	1.46
1	A	128	ARG	NE-CZ	5.57	1.40	1.33
1	A	12	PRO	N-CD	5.55	1.55	1.47
1	A	170	TYR	CZ-OH	5.46	1.47	1.37
1	A	130	TRP	CZ3-CH2	5.39	1.48	1.40
1	A	129	GLY	N-CA	-5.36	1.38	1.46
1	A	231	ILE	C-O	5.36	1.33	1.23
1	A	77	LYS	CA-CB	-5.34	1.42	1.53
1	A	33	PHE	CE2-CZ	5.28	1.47	1.37
1	A	296	GLU	CG-CD	5.28	1.59	1.51
1	A	269	ASN	CB-CG	5.23	1.63	1.51
1	A	287	VAL	CB-CG2	5.23	1.63	1.52
1	A	194	PRO	N-CD	5.21	1.55	1.47
1	A	126	GLN	N-CA	5.21	1.56	1.46
1	A	297	GLU	CD-OE2	-5.18	1.20	1.25
1	A	67	ASP	N-CA	5.17	1.56	1.46
1	A	170	TYR	CG-CD1	5.17	1.45	1.39
1	A	130	TRP	NE1-CE2	5.16	1.44	1.37
1	A	19	THR	CB-OG1	5.15	1.53	1.43
1	A	120	GLU	CG-CD	5.12	1.59	1.51
1	A	127	LYS	C-N	5.08	1.45	1.34
1	A	35	VAL	CA-CB	5.03	1.65	1.54
1	A	12	PRO	C-N	-5.01	1.22	1.34

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NE-CZ-NH1	43.97	142.29	120.30
1	A	291	ARG	NE-CZ-NH1	23.36	131.98	120.30
1	A	150	ARG	NE-CZ-NH2	-20.13	110.23	120.30
1	A	79	ARG	CD-NE-CZ	20.08	151.71	123.60
1	A	149	ARG	NE-CZ-NH2	-19.73	110.44	120.30
1	A	235	ASP	CB-CG-OD1	16.00	132.70	118.30
1	A	116	ARG	NE-CZ-NH1	14.25	127.43	120.30
1	A	79	ARG	NH1-CZ-NH2	-13.92	104.09	119.40
1	A	67	ASP	CB-CG-OD2	-13.72	105.95	118.30
1	A	292	ASP	CB-CG-OD2	-13.68	105.99	118.30
1	A	124	GLU	OE1-CD-OE2	13.49	139.49	123.30
1	A	79	ARG	NE-CZ-NH2	-13.40	113.60	120.30
1	A	291	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	A	296	GLU	OE1-CD-OE2	12.58	138.39	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	TYR	CB-CG-CD2	-12.48	113.51	121.00
1	A	67	ASP	CB-CG-OD1	12.40	129.46	118.30
1	A	123	LYS	CA-CB-CG	12.23	140.30	113.40
1	A	115	GLU	OE1-CD-OE2	11.85	137.52	123.30
1	A	276	GLU	OE1-CD-OE2	11.46	137.06	123.30
1	A	214	ARG	NE-CZ-NH2	11.12	125.86	120.30
1	A	120	GLU	OE1-CD-OE2	10.50	135.90	123.30
1	A	54	ALA	N-CA-CB	-10.19	95.84	110.10
1	A	81	TYR	CB-CG-CD1	-10.02	114.99	121.00
1	A	170	TYR	CB-CG-CD1	-9.65	115.21	121.00
1	A	268	TYR	CG-CD1-CE1	-9.33	113.84	121.30
1	A	249	TYR	O-C-N	-9.28	107.42	123.20
1	A	287	VAL	CG1-CB-CG2	-9.26	96.09	110.90
1	A	150	ARG	NH1-CZ-NH2	9.17	129.49	119.40
1	A	79	ARG	CG-CD-NE	9.01	130.73	111.80
1	A	151	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	A	81	TYR	CB-CG-CD2	8.88	126.33	121.00
1	A	257	ASP	CB-CG-OD1	8.82	126.24	118.30
1	A	131	ASP	CB-CG-OD1	8.62	126.06	118.30
1	A	130	TRP	CB-CG-CD2	-8.56	115.47	126.60
1	A	170	TYR	CB-CG-CD2	8.52	126.11	121.00
1	A	25	ASP	CB-CG-OD1	8.51	125.96	118.30
1	A	79	ARG	CA-CB-CG	8.41	131.90	113.40
1	A	150	ARG	CA-CB-CG	-8.32	95.09	113.40
1	A	130	TRP	CB-CG-CD1	8.31	137.81	127.00
1	A	34	GLU	OE1-CD-OE2	8.23	133.18	123.30
1	A	131	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	A	268	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	A	17	PHE	CB-CG-CD2	-7.89	115.27	120.80
1	A	22	LYS	CA-CB-CG	7.53	129.97	113.40
1	A	44	GLU	OE1-CD-OE2	7.45	132.24	123.30
1	A	274	ASP	CB-CG-OD1	7.44	125.00	118.30
1	A	128	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	292	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	294	PHE	CB-CG-CD1	-7.19	115.77	120.80
1	A	302	GLY	O-C-N	-7.14	111.28	122.70
1	A	102	THR	OG1-CB-CG2	7.06	126.23	110.00
1	A	82	ASP	N-CA-CB	7.05	123.30	110.60
1	A	268	TYR	CD1-CG-CD2	7.01	125.61	117.90
1	A	239	GLU	OE1-CD-OE2	-6.97	114.93	123.30
1	A	235	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	12	PRO	N-CD-CG	-6.86	92.91	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	LEU	CB-CG-CD1	6.84	122.62	111.00
1	A	77	LYS	CA-CB-CG	6.79	128.34	113.40
1	A	122	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	A	296	GLU	CG-CD-OE2	-6.78	104.75	118.30
1	A	61	PHE	CB-CG-CD1	-6.74	116.08	120.80
1	A	195	GLU	OE1-CD-OE2	-6.74	115.21	123.30
1	A	101	ASP	CA-CB-CG	-6.70	98.67	113.40
1	A	122	TYR	CG-CD2-CE2	-6.68	115.96	121.30
1	A	116	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	122	TYR	CD1-CE1-CZ	-6.64	113.82	119.80
1	A	134	GLU	OE1-CD-OE2	6.60	131.22	123.30
1	A	149	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	300	LYS	CA-CB-CG	6.57	127.86	113.40
1	A	7	PHE	CG-CD2-CE2	-6.53	113.61	120.80
1	A	167	LYS	C-N-CA	-6.53	105.37	121.70
1	A	44	GLU	CA-CB-CG	-6.47	99.16	113.40
1	A	146	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	101	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	125	MET	CA-CB-CG	-6.47	102.30	113.30
1	A	183	PHE	CG-CD2-CE2	-6.46	113.69	120.80
1	A	4	LYS	CA-CB-CG	-6.45	99.20	113.40
1	A	167	LYS	O-C-N	6.43	132.99	122.70
1	A	285	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	79	ARG	CB-CG-CD	6.42	128.29	111.60
1	A	249	TYR	CD1-CG-CD2	6.41	124.95	117.90
1	A	102	THR	CA-CB-CG2	-6.41	103.43	112.40
1	A	119	GLN	CG-CD-OE1	6.37	134.35	121.60
1	A	145	LEU	O-C-N	-6.34	112.55	122.70
1	A	13	GLU	CG-CD-OE1	6.33	130.97	118.30
1	A	296	GLU	CB-CG-CD	-6.32	97.15	114.20
1	A	157	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	182	ALA	O-C-N	-6.28	112.65	122.70
1	A	199	TRP	CD1-NE1-CE2	-6.27	103.36	109.00
1	A	282	GLU	OE1-CD-OE2	6.26	130.81	123.30
1	A	45	LYS	O-C-N	-6.22	112.75	122.70
1	A	13	GLU	CG-CD-OE2	-6.21	105.88	118.30
1	A	124	GLU	O-C-N	-6.21	112.77	122.70
1	A	31	LEU	O-C-N	-6.20	112.67	123.20
1	A	206	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	191	VAL	O-C-N	6.15	132.54	122.70
1	A	262	LYS	CA-CB-CG	-6.15	99.87	113.40
1	A	25	ASP	CB-CG-OD2	-6.15	112.77	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	GLU	CG-CD-OE1	-6.09	106.11	118.30
1	A	291	ARG	O-C-N	6.06	132.40	122.70
1	A	220	GLY	CA-C-O	-6.03	109.75	120.60
1	A	249	TYR	CA-C-N	6.01	128.22	116.20
1	A	149	ARG	NH1-CZ-NH2	5.95	125.94	119.40
1	A	193	HIS	CA-CB-CG	-5.93	103.51	113.60
1	A	236	ALA	N-CA-CB	-5.92	101.81	110.10
1	A	77	LYS	CG-CD-CE	-5.91	94.18	111.90
1	A	178	ASP	O-C-N	5.87	132.09	122.70
1	A	211	GLY	O-C-N	-5.79	113.35	123.20
1	A	164	PHE	CD1-CE1-CZ	-5.78	113.16	120.10
1	A	257	ASP	OD1-CG-OD2	-5.77	112.33	123.30
1	A	40	VAL	CA-CB-CG2	5.77	119.55	110.90
1	A	98	LYS	CA-CB-CG	5.76	126.06	113.40
1	A	29	LYS	CB-CA-C	-5.75	98.90	110.40
1	A	273	LYS	CD-CE-NZ	5.74	124.91	111.70
1	A	300	LYS	CB-CA-C	-5.74	98.92	110.40
1	A	271	VAL	CA-CB-CG1	5.72	119.49	110.90
1	A	5	LEU	CA-C-O	-5.71	108.11	120.10
1	A	76	ALA	CA-C-N	5.64	129.60	117.20
1	A	105	LEU	O-C-N	5.62	131.70	122.70
1	A	232	ASN	O-C-N	5.62	132.76	123.20
1	A	191	VAL	CA-C-O	-5.61	108.32	120.10
1	A	4	LYS	CD-CE-NZ	-5.61	98.80	111.70
1	A	268	TYR	CG-CD2-CE2	-5.59	116.83	121.30
1	A	214	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	287	VAL	CA-CB-CG1	5.54	119.21	110.90
1	A	195	GLU	CG-CD-OE2	5.53	129.36	118.30
1	A	67	ASP	N-CA-CB	-5.52	100.66	110.60
1	A	183	PHE	CZ-CE2-CD2	5.50	126.69	120.10
1	A	237	VAL	CA-C-O	-5.49	108.58	120.10
1	A	67	ASP	CA-CB-CG	-5.46	101.38	113.40
1	A	69	LYS	CA-CB-CG	-5.45	101.40	113.40
1	A	109	ALA	N-CA-CB	-5.45	102.47	110.10
1	A	120	GLU	CG-CD-OE2	-5.45	107.41	118.30
1	A	274	ASP	CA-C-O	5.41	131.46	120.10
1	A	211	GLY	C-N-CA	5.41	133.65	122.30
1	A	274	ASP	O-C-N	-5.38	114.08	122.70
1	A	100	MET	C-N-CA	5.38	135.14	121.70
1	A	268	TYR	CA-C-O	-5.37	108.82	120.10
1	A	166	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	A	145	LEU	CA-C-O	5.34	131.31	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	GLU	CB-CA-C	-5.31	99.79	110.40
1	A	14	GLU	CB-CA-C	-5.30	99.81	110.40
1	A	33	PHE	CG-CD2-CE2	5.28	126.61	120.80
1	A	90	ASP	N-CA-CB	-5.28	101.11	110.60
1	A	17	PHE	CG-CD1-CE1	-5.27	115.00	120.80
1	A	182	ALA	N-CA-CB	-5.25	102.75	110.10
1	A	122	TYR	CD1-CG-CD2	5.19	123.60	117.90
1	A	130	TRP	N-CA-CB	-5.19	101.26	110.60
1	A	22	LYS	CB-CG-CD	-5.18	98.14	111.60
1	A	147	THR	CA-CB-OG1	-5.15	98.18	109.00
1	A	240	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	A	201	ILE	CA-CB-CG1	-5.14	101.23	111.00
1	A	249	TYR	CA-CB-CG	-5.14	103.63	113.40
1	A	248	PHE	O-C-N	5.12	130.89	122.70
1	A	30	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	96	LYS	CG-CD-CE	5.11	127.23	111.90
1	A	237	VAL	CA-CB-CG1	-5.10	103.25	110.90
1	A	143	ASN	N-CA-CB	-5.07	101.47	110.60
1	A	138	MET	CB-CG-SD	-5.06	97.21	112.40
1	A	249	TYR	N-CA-CB	-5.06	101.49	110.60
1	A	301	LYS	CB-CG-CD	5.05	124.73	111.60
1	A	34	GLU	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2316	0	2325	30	0
2	A	12	0	12	0	0
3	A	12	0	11	1	0
4	A	236	0	0	10	1
All	All	2576	0	2348	30	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:ASP:HB2	4:A:503:HOH:O	1.45	1.16
1:A:276:GLU:OE1	1:A:276:GLU:HA	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:69:LYS:NZ	4:A:490:HOH:O	1.80	0.75
1:A:146:ASP:CB	4:A:503:HOH:O	2.18	0.71
1:A:296:GLU:CD	4:A:416:HOH:O	2.29	0.71
1:A:160:LYS:HD3	1:A:166:GLU:HG2	1.78	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:273:LYS:O	1:A:275:VAL:HG23	2.00	0.61
1:A:143:ASN:OD1	1:A:149:ARG:HG3	2.00	0.60
1:A:84:LYS:HD2	1:A:270:TRP:CE2	2.36	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:273:LYS:O	1:A:274:ASP:C	2.41	0.59
1:A:306:LYS:C	4:A:494:HOH:O	2.41	0.57
1:A:69:LYS:CE	4:A:490:HOH:O	2.42	0.54
1:A:131:ASP:OD1	1:A:133:LYS:HG3	2.09	0.52
1:A:172:VAL:HB	1:A:189:MET:HE3	1.94	0.49
1:A:123:LYS:O	1:A:127:LYS:NZ	2.46	0.47
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:293:ASN:C	1:A:293:ASN:OD1	2.57	0.42
1:A:146:ASP:CG	4:A:503:HOH:O	2.50	0.41
1:A:25:ASP:O	1:A:29:LYS:HG3	2.21	0.41
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.85	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	Distance(Å)	Clash(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%)	30 13

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%)	235 (97%)	8 (3%)	50 30

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	59	LYS
1	A	98	LYS
1	A	99	PRO
1	A	127	LYS
1	A	204	MET
1	A	276	GLU
1	A	299	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	GLA	A	307[A]	-	12,12,12	1.50	3 (25%)	17,17,17	1.52	4 (23%)
3	GAL	A	308[B]	-	12,12,12	1.77	2 (16%)	17,17,17	1.67	1 (5%)

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	GLA	A	307[A]	-	-	0/2/22/22	0/1/1/1
3	GAL	A	308[B]	-	-	0/2/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	308[B]	GAL	C3-C2	-5.07	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	307[A]	GLA	O2-C2	2.59	1.49	1.43
3	A	308[B]	GAL	C4-C3	2.55	1.59	1.52
2	A	307[A]	GLA	O5-C1	2.39	1.47	1.43
2	A	307[A]	GLA	C1-C2	-2.03	1.49	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	308[B]	GAL	O3-C3-C2	4.27	119.92	110.35
2	A	307[A]	GLA	O4-C4-C5	2.67	116.32	109.28
2	A	307[A]	GLA	O5-C5-C6	-2.31	100.67	106.34
2	A	307[A]	GLA	C1-O5-C5	-2.14	109.57	113.40
2	A	307[A]	GLA	O6-C6-C5	-2.08	104.19	111.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.