



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:22 PM UTC

PDB ID : 7ABP / pdb_00007abp
Title : SUGAR-BINDING AND CRYSTALLOGRAPHIC STUDIES OF AN ARABINOSE-BINDING PROTEIN MUTANT (MET108LEU) WHICH EXHIBITS ENHANCED AFFINITY AND ALTERED SPECIFICITY
Authors : Vermersch, P.S.; Tesmer, J.J.G.; Quijcho, F.A.
Deposited on : 1991-04-25
Resolution : 1.67 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

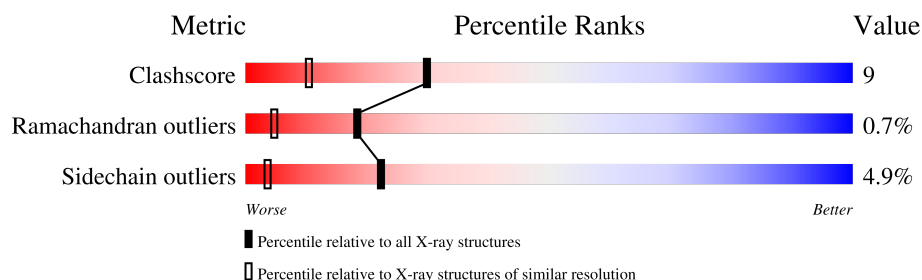
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)

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	 62% 31% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2531 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.

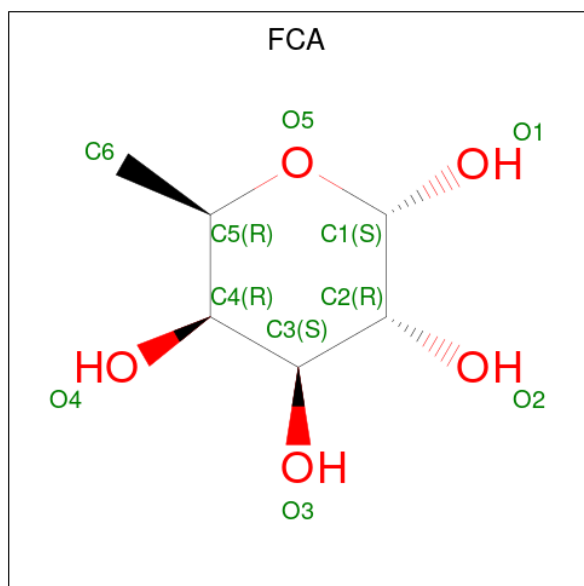
- Molecule 1 is a protein called L-ARABINOSE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2316	1474	389	443	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

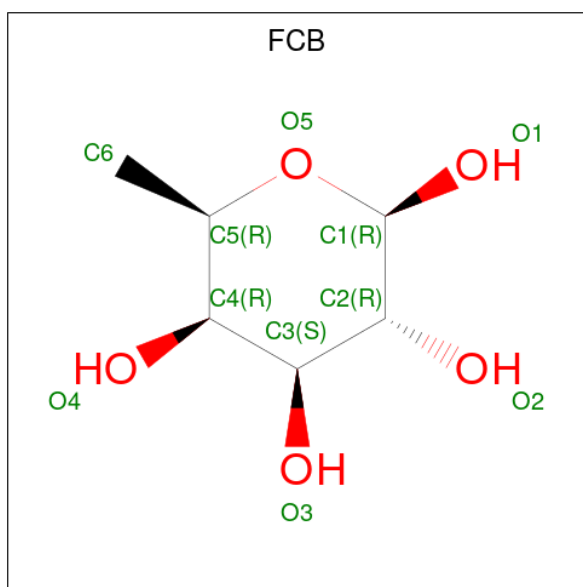
Chain	Residue	Modelled	Actual	Comment	Reference
A	108	LEU	MET	conflict	UNP P02924

- Molecule 2 is alpha-D-fucopyranose (CCD ID: FCA) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	11	6	5	0	1

- Molecule 3 is beta-D-fucopyranose (CCD ID: FCB) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			11	6	5		

- Molecule 4 is water.

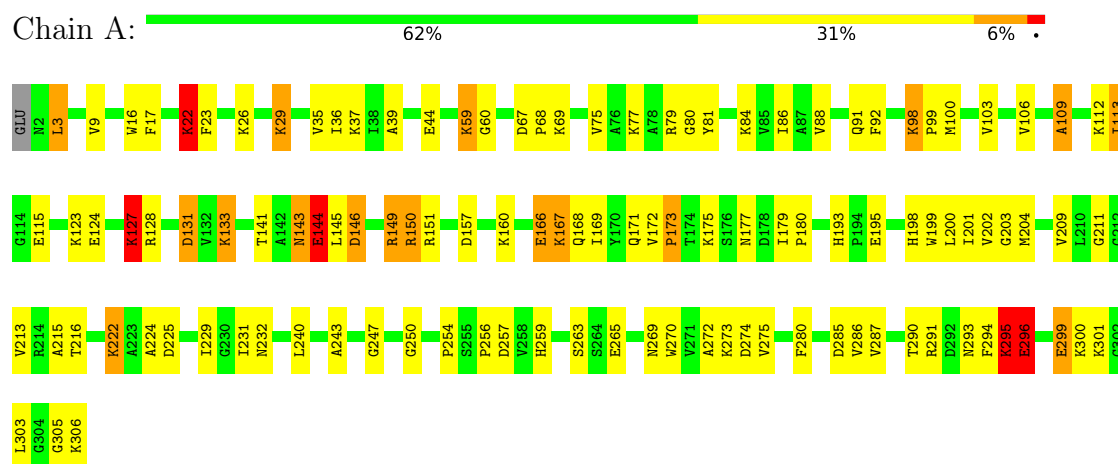
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		

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



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	55.75Å 71.83Å 78.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.67	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.67)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2531	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FCA, FCB

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	1.66	19/2361 (0.8%)	2.33	144/3190 (4.5%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	VAL	C-O	10.05	1.33	1.24
1	A	203	GLY	N-CA	9.02	1.54	1.45
1	A	250	GLY	N-CA	8.36	1.54	1.45
1	A	231	ILE	C-O	8.33	1.32	1.24
1	A	106	VAL	C-O	6.46	1.31	1.24
1	A	200	LEU	C-O	6.14	1.31	1.24
1	A	263	SER	N-CA	6.13	1.53	1.46
1	A	201	ILE	C-O	5.91	1.30	1.24
1	A	280	PHE	C-O	5.74	1.30	1.23
1	A	259	HIS	N-CA	5.66	1.53	1.46
1	A	86	ILE	C-O	5.63	1.29	1.24
1	A	231	ILE	C-N	-5.53	1.25	1.33
1	A	16	TRP	C-O	5.41	1.30	1.24
1	A	305	GLY	CA-C	5.25	1.55	1.52
1	A	9	VAL	N-CA	5.24	1.52	1.46
1	A	88	VAL	C-N	-5.16	1.26	1.33
1	A	36	ILE	C-O	5.13	1.29	1.24
1	A	157	ASP	C-O	5.07	1.30	1.24
1	A	23	PHE	N-CA	5.05	1.52	1.46

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	GLU	N-CA-CB	9.52	123.81	110.01
1	A	222	LYS	CA-C-N	9.44	133.31	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	LYS	C-N-CA	9.44	133.31	120.38
1	A	295	LYS	CA-C-O	-9.12	110.75	120.42
1	A	92	PHE	CA-CB-CG	8.76	122.56	113.80
1	A	193	HIS	CA-CB-CG	-8.74	105.06	113.80
1	A	285	ASP	CA-CB-CG	8.62	121.22	112.60
1	A	99	PRO	CA-C-O	-8.44	112.12	121.32
1	A	231	ILE	CA-C-N	8.42	137.62	121.54
1	A	231	ILE	C-N-CA	8.42	137.62	121.54
1	A	213	VAL	CA-C-O	-8.41	112.26	121.17
1	A	259	HIS	O-C-N	-8.36	113.46	122.07
1	A	296	GLU	CA-CB-CG	8.30	130.71	114.10
1	A	200	LEU	CA-C-O	-8.23	111.46	120.43
1	A	149	ARG	NE-CZ-NH1	-8.01	113.49	121.50
1	A	231	ILE	CA-C-O	-7.97	111.91	120.36
1	A	39	ALA	CA-C-O	-7.95	111.56	120.54
1	A	109	ALA	CA-C-N	7.92	131.80	120.79
1	A	109	ALA	C-N-CA	7.92	131.80	120.79
1	A	296	GLU	CB-CA-C	-7.91	98.46	110.88
1	A	79	ARG	CA-CB-CG	7.90	129.90	114.10
1	A	300	LYS	N-CA-CB	7.38	120.97	110.12
1	A	151	ARG	NE-CZ-NH1	7.35	128.85	121.50
1	A	29	LYS	N-CA-CB	7.23	120.75	110.12
1	A	16	TRP	O-C-N	-7.23	114.57	122.09
1	A	98	LYS	CA-C-N	7.23	127.66	119.93
1	A	98	LYS	C-N-CA	7.23	127.66	119.93
1	A	44	GLU	CB-CG-CD	7.21	124.86	112.60
1	A	263	SER	CA-C-N	7.19	129.79	120.44
1	A	263	SER	C-N-CA	7.19	129.79	120.44
1	A	99	PRO	CB-CA-C	-6.96	102.81	111.64
1	A	113	ILE	CB-CG1-CD1	6.95	128.39	113.80
1	A	17	PHE	CA-CB-CG	-6.80	107.00	113.80
1	A	131	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	296	GLU	O-C-N	6.73	129.00	122.07
1	A	149	ARG	CA-C-O	-6.70	113.45	120.55
1	A	299	GLU	CA-C-O	-6.68	113.33	120.42
1	A	202	VAL	CA-C-O	-6.65	113.45	120.57
1	A	286	VAL	O-C-N	6.62	129.54	123.19
1	A	203	GLY	N-CA-C	-6.62	99.23	111.14
1	A	150	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	A	247	GLY	N-CA-C	-6.58	106.19	114.16
1	A	215	ALA	O-C-N	-6.57	115.16	122.12
1	A	88	VAL	CA-C-N	6.53	134.01	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	VAL	C-N-CA	6.53	134.01	121.54
1	A	133	LYS	CA-C-N	-6.43	112.44	122.67
1	A	133	LYS	C-N-CA	-6.43	112.44	122.67
1	A	115	GLU	CA-C-O	-6.39	113.77	120.55
1	A	106	VAL	CA-C-O	-6.39	113.74	120.39
1	A	3	LEU	CA-C-O	-6.37	113.43	120.69
1	A	303	LEU	CA-C-N	6.35	133.86	121.41
1	A	303	LEU	C-N-CA	6.35	133.86	121.41
1	A	291	ARG	NE-CZ-NH1	6.35	127.85	121.50
1	A	216	THR	CA-CB-OG1	-6.31	100.14	109.60
1	A	229	ILE	CA-C-N	-6.25	116.09	122.27
1	A	229	ILE	C-N-CA	-6.25	116.09	122.27
1	A	225	ASP	CA-CB-CG	-6.22	106.38	112.60
1	A	195	GLU	CA-C-N	-6.19	113.12	121.66
1	A	195	GLU	C-N-CA	-6.19	113.12	121.66
1	A	103	VAL	O-C-N	6.12	126.90	121.57
1	A	151	ARG	CA-C-O	-6.10	114.42	120.70
1	A	243	ALA	CA-C-O	6.08	126.96	120.70
1	A	22	LYS	CA-CB-CG	6.08	126.25	114.10
1	A	247	GLY	CA-C-O	-6.07	112.34	119.50
1	A	143	ASN	CA-CB-CG	-6.05	106.55	112.60
1	A	193	HIS	N-CA-C	6.05	119.59	108.94
1	A	69	LYS	O-C-N	-6.04	114.12	122.46
1	A	168	GLN	OE1-CD-NE2	-6.04	116.56	122.60
1	A	300	LYS	CB-CA-C	-6.00	100.83	110.79
1	A	286	VAL	CA-C-O	-6.00	115.32	120.96
1	A	173	PRO	N-CA-CB	5.98	108.87	103.19
1	A	124	GLU	O-C-N	-5.97	115.34	122.15
1	A	145	LEU	O-C-N	-5.95	115.97	123.05
1	A	79	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	A	103	VAL	CA-C-O	-5.86	115.69	119.15
1	A	177	ASN	CA-C-O	-5.82	115.12	122.63
1	A	79	ARG	CG-CD-NE	5.80	124.77	112.00
1	A	193	HIS	CA-C-N	5.78	125.46	119.56
1	A	193	HIS	C-N-CA	5.78	125.46	119.56
1	A	23	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	29	LYS	CB-CA-C	-5.77	101.21	110.79
1	A	143	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	166	GLU	N-CA-C	5.75	118.32	111.71
1	A	265	GLU	CA-C-N	5.70	128.39	120.29
1	A	265	GLU	C-N-CA	5.70	128.39	120.29
1	A	240	LEU	CA-C-N	5.67	131.07	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	LEU	C-N-CA	5.67	131.07	121.14
1	A	145	LEU	CA-C-O	5.65	126.41	120.54
1	A	141	THR	N-CA-C	5.64	118.91	109.95
1	A	150	ARG	CA-CB-CG	-5.64	102.83	114.10
1	A	269	ASN	O-C-N	5.63	128.81	122.22
1	A	222	LYS	O-C-N	-5.63	116.09	122.68
1	A	274	ASP	N-CA-CB	5.62	119.98	110.49
1	A	3	LEU	O-C-N	5.60	129.59	123.04
1	A	150	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	A	128	ARG	CA-C-N	5.57	130.84	120.87
1	A	128	ARG	C-N-CA	5.57	130.84	120.87
1	A	144	GLU	CB-CG-CD	5.57	122.07	112.60
1	A	36	ILE	CB-CA-C	5.57	117.70	110.96
1	A	259	HIS	CA-C-N	5.56	126.00	119.94
1	A	259	HIS	C-N-CA	5.56	126.00	119.94
1	A	263	SER	O-C-N	-5.55	116.23	122.12
1	A	127	LYS	O-C-N	-5.50	116.28	122.12
1	A	22	LYS	CB-CG-CD	-5.50	98.64	111.30
1	A	75	VAL	CA-C-O	-5.47	115.38	121.17
1	A	79	ARG	N-CA-CB	5.45	118.13	110.12
1	A	296	GLU	CA-C-O	-5.45	115.10	120.82
1	A	169	ILE	CA-C-O	-5.42	114.31	120.66
1	A	22	LYS	CG-CD-CE	-5.38	98.93	111.30
1	A	300	LYS	CA-C-O	-5.38	114.85	120.55
1	A	216	THR	CA-C-N	5.36	127.40	120.44
1	A	216	THR	C-N-CA	5.36	127.40	120.44
1	A	141	THR	CA-CB-OG1	-5.35	101.57	109.60
1	A	256	PRO	O-C-N	-5.34	115.33	122.22
1	A	144	GLU	CG-CD-OE1	5.34	130.68	118.40
1	A	81	TYR	CA-C-O	-5.32	113.34	119.56
1	A	60	GLY	N-CA-C	-5.30	102.52	110.42
1	A	35	VAL	CA-C-O	-5.26	114.85	120.59
1	A	209	VAL	CA-C-O	-5.26	115.27	120.85
1	A	293	ASN	N-CA-CB	-5.24	102.99	110.80
1	A	167	LYS	CA-C-N	-5.23	114.85	122.86
1	A	167	LYS	C-N-CA	-5.23	114.85	122.86
1	A	295	LYS	O-C-N	5.23	128.12	122.15
1	A	67	ASP	CA-C-O	-5.23	113.00	120.16
1	A	149	ARG	CD-NE-CZ	5.21	131.69	124.40
1	A	243	ALA	O-C-N	-5.20	116.47	122.09
1	A	259	HIS	CA-CB-CG	5.19	118.99	113.80
1	A	131	ASP	CA-C-O	-5.19	114.56	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	287	VAL	CA-CB-CG1	5.15	119.15	110.40
1	A	294	PHE	CA-C-O	-5.14	115.10	120.55
1	A	199	TRP	CA-C-O	-5.13	115.16	120.70
1	A	211	GLY	O-C-N	-5.13	117.26	122.19
1	A	100	MET	CA-CB-CG	-5.13	103.85	114.10
1	A	151	ARG	CG-CD-NE	-5.12	100.73	112.00
1	A	211	GLY	CA-C-N	5.12	125.62	119.94
1	A	211	GLY	C-N-CA	5.12	125.62	119.94
1	A	77	LYS	O-C-N	5.12	127.54	122.12
1	A	198	HIS	O-C-N	5.07	129.54	123.36
1	A	198	HIS	CA-C-O	-5.05	114.07	120.28
1	A	146	ASP	O-C-N	5.03	127.32	122.09
1	A	80	GLY	CA-C-N	-5.03	114.60	122.65
1	A	80	GLY	C-N-CA	-5.03	114.60	122.65
1	A	171	GLN	O-C-N	5.00	129.56	123.21

There are no chirality outliers.

There are no planarity outliers.

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	2316	0	2328	40	0
2	A	11	0	12	0	0
3	A	11	0	11	0	0
4	A	193	0	0	5	0
All	All	2531	0	2351	40	0

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 9.

All (40) 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:127:LYS:HB2	1:A:127:LYS:NZ	1.22	1.16
1:A:127:LYS:HZ3	1:A:127:LYS:CB	1.61	1.07
1:A:127:LYS:NZ	1:A:127:LYS:CB	2.07	1.00
1:A:160:LYS:HD3	1:A:166:GLU:HG2	1.48	0.95
1:A:127:LYS:HB2	1:A:127:LYS:HZ2	1.33	0.94
1:A:131:ASP:OD2	1:A:133:LYS:HG3	1.91	0.70
1:A:295:LYS:NZ	1:A:306:LYS:O	2.27	0.67
1:A:127:LYS:CB	1:A:127:LYS:HZ2	1.93	0.66
1:A:127:LYS:HE2	4:A:359:HOH:O	1.98	0.64
1:A:3:LEU:HD12	1:A:59:LYS:HG2	1.81	0.62
1:A:146:ASP:O	1:A:150:ARG:HG3	2.01	0.60
1:A:167:LYS:HG2	4:A:426:HOH:O	2.02	0.59
1:A:160:LYS:CD	1:A:166:GLU:HG2	2.27	0.59
1:A:273:LYS:HB2	1:A:275:VAL:HG23	1.87	0.57
1:A:3:LEU:CD1	1:A:59:LYS:CG	2.83	0.56
1:A:144:GLU:H	1:A:144:GLU:CD	2.15	0.55
1:A:3:LEU:CD1	1:A:59:LYS:HG2	2.38	0.53
1:A:109:ALA:O	1:A:113:ILE:HD12	2.09	0.52
1:A:3:LEU:CD1	1:A:59:LYS:HG3	2.40	0.51
1:A:59:LYS:HB3	1:A:59:LYS:HZ2	1.75	0.51
1:A:127:LYS:HB2	1:A:127:LYS:HZ3	0.69	0.51
1:A:68:PRO:HB3	1:A:91:GLN:O	2.11	0.51
1:A:272:ALA:C	1:A:273:LYS:HG3	2.36	0.49
1:A:84:LYS:HE2	4:A:479:HOH:O	2.12	0.49
1:A:3:LEU:HD11	1:A:59:LYS:CG	2.45	0.47
1:A:257:ASP:OD2	1:A:301:LYS:NZ	2.46	0.47
1:A:296:GLU:CD	4:A:402:HOH:O	2.58	0.47
1:A:222:LYS:HE2	1:A:224:ALA:HB3	1.95	0.46
1:A:84:LYS:HD2	1:A:270:TRP:CZ2	2.53	0.43
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.98	0.43
1:A:22:LYS:HB2	1:A:22:LYS:HE2	1.13	0.42
1:A:295:LYS:CE	1:A:306:LYS:O	2.67	0.42
1:A:3:LEU:HD12	1:A:59:LYS:CG	2.44	0.42
1:A:172:VAL:HA	1:A:173:PRO:HD3	1.91	0.42
1:A:3:LEU:HD11	1:A:59:LYS:HG3	2.01	0.42
1:A:143:ASN:OD1	1:A:149:ARG:HG3	2.20	0.42
1:A:295:LYS:CD	4:A:450:HOH:O	2.68	0.41
1:A:84:LYS:HD2	1:A:270:TRP:CE2	2.55	0.41
1:A:112:LYS:HD3	1:A:112:LYS:HA	1.59	0.41
1:A:26:LYS:HA	1:A:29:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.

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%)	296 (98%)	5 (2%)	2 (1%)	18 5

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%)	231 (95%)	12 (5%)	22 3

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	37	LYS
1	A	59	LYS
1	A	98	LYS
1	A	123	LYS
1	A	127	LYS
1	A	144	GLU
1	A	175	LYS
1	A	204	MET

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Mol	Chain	Res	Type
1	A	295	LYS
1	A	296	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	244	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 ⓘ

There are no oligosaccharides 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	FCA	A	307[A]	-	11,11,11	1.05	0	16,16,16	1.75	2 (12%)
3	FCB	A	308[B]	-	11,11,11	2.39	3 (27%)	16,16,16	1.64	3 (18%)

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	FCA	A	307[A]	-	-	-	0/1/1/1
3	FCB	A	308[B]	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	308[B]	FCB	C3-C2	-6.23	1.36	1.52
3	A	308[B]	FCB	O3-C3	3.32	1.51	1.43
3	A	308[B]	FCB	C4-C3	3.18	1.60	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	307[A]	FCA	C1-O5-C5	5.35	122.70	114.37
3	A	308[B]	FCB	O3-C3-C4	-3.46	102.22	110.38
3	A	308[B]	FCB	O3-C3-C2	2.86	117.11	110.38
3	A	308[B]	FCB	C4-C3-C2	2.59	115.37	110.83
2	A	307[A]	FCA	C1-C2-C3	2.12	114.68	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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.