



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:15 PM UTC

PDB ID : 1ABF / pdb_00001abf
Title : SUBSTRATE SPECIFICITY AND AFFINITY OF A PROTEIN MODULATED BY BOUND WATER MOLECULES
Authors : Wilson, D.K.; Quioco, F.A.
Deposited on : 1992-04-23
Resolution : 1.90 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

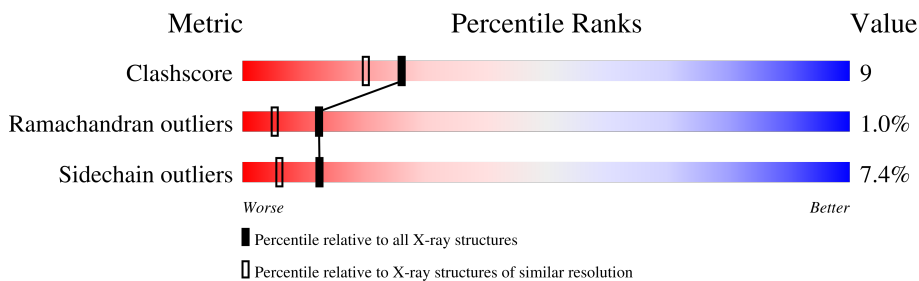
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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](#)

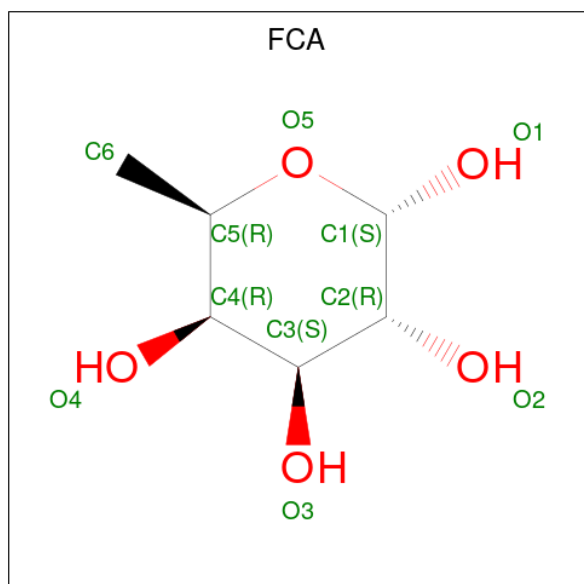
There are 4 unique types of molecules in this entry. The entry contains 2528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

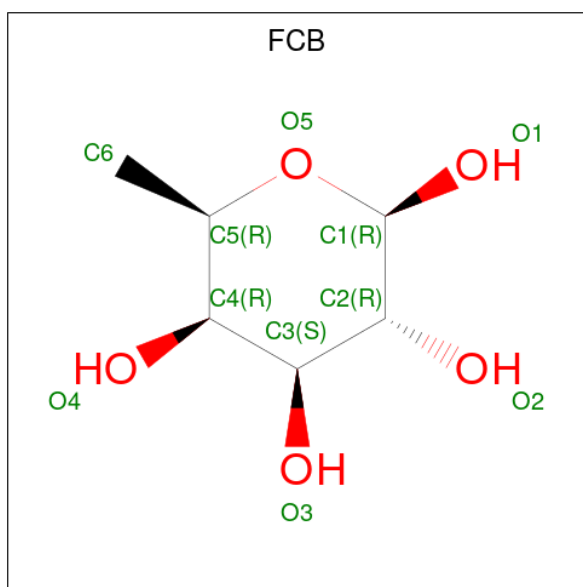
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2315	1473	388	443	11	0	0	0

- 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.

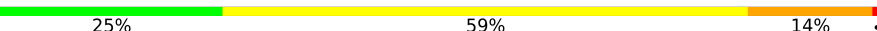
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total	O	0	0
			191	191		

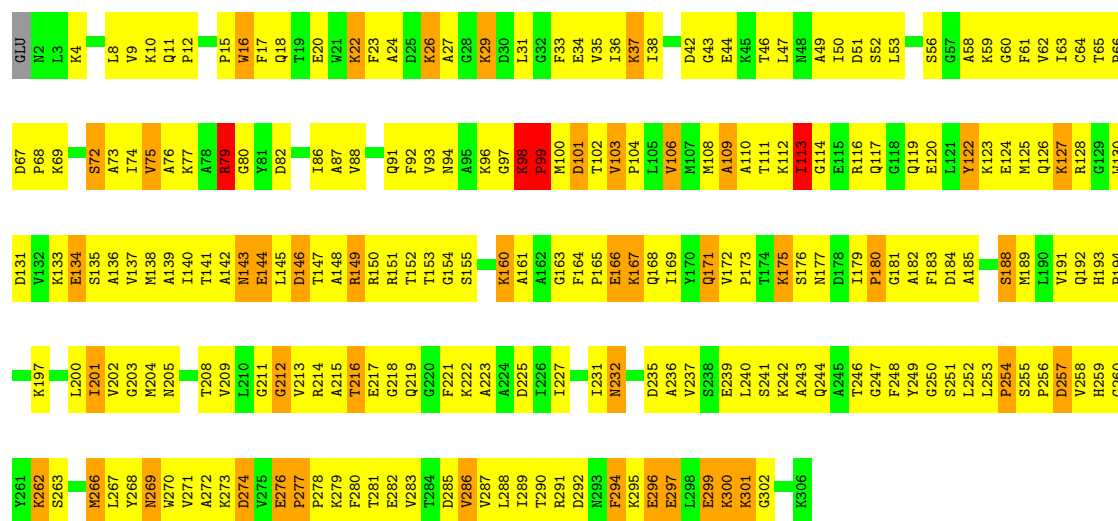
3 Residue-property plots

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 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.134 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2528	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	2.76	172/2360 (7.3%)	2.95	289/3188 (9.1%)

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	LEU	N-CA	10.94	1.59	1.46
1	A	88	VAL	C-O	10.78	1.35	1.24
1	A	103	VAL	CA-C	10.58	1.61	1.53
1	A	259	HIS	N-CA	10.35	1.58	1.46
1	A	86	ILE	C-O	9.89	1.33	1.24
1	A	214	ARG	NE-CZ	9.89	1.44	1.33
1	A	94	ASN	N-CA	9.60	1.57	1.46
1	A	63	ILE	CA-CB	9.51	1.68	1.54
1	A	297	GLU	C-O	9.49	1.35	1.24
1	A	60	GLY	N-CA	9.46	1.56	1.45
1	A	176	SER	CA-C	9.27	1.63	1.52
1	A	297	GLU	CA-C	-9.05	1.41	1.52
1	A	181	GLY	CA-C	-8.99	1.42	1.52
1	A	263	SER	N-CA	8.73	1.56	1.46
1	A	10	LYS	C-N	8.72	1.45	1.33
1	A	256	PRO	C-N	8.50	1.45	1.33
1	A	87	ALA	N-CA	-8.32	1.34	1.46
1	A	9	VAL	C-O	8.31	1.32	1.24
1	A	146	ASP	C-O	-8.28	1.14	1.24
1	A	49	ALA	N-CA	8.23	1.56	1.46
1	A	106	VAL	C-O	8.22	1.33	1.24
1	A	202	VAL	C-N	-7.92	1.23	1.33
1	A	248	PHE	CA-C	7.86	1.62	1.52
1	A	80	GLY	CA-C	-7.81	1.42	1.52
1	A	116	ARG	CD-NE	7.75	1.57	1.46
1	A	136	ALA	CA-C	-7.72	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	LYS	C-N	-7.66	1.24	1.33
1	A	231	ILE	C-O	7.62	1.31	1.24
1	A	86	ILE	CA-C	-7.60	1.43	1.52
1	A	260	GLY	CA-C	-7.51	1.43	1.52
1	A	130	TRP	C-O	7.42	1.32	1.23
1	A	88	VAL	N-CA	7.33	1.54	1.46
1	A	111	THR	CA-C	7.17	1.62	1.52
1	A	249	TYR	C-O	7.07	1.32	1.24
1	A	177	ASN	C-N	-7.06	1.24	1.33
1	A	250	GLY	C-N	-7.06	1.24	1.33
1	A	194	PRO	N-CA	-7.04	1.38	1.47
1	A	36	ILE	C-O	7.04	1.32	1.23
1	A	282	GLU	C-O	7.03	1.32	1.24
1	A	277	PRO	CA-C	-6.96	1.45	1.52
1	A	35	VAL	C-N	-6.95	1.25	1.33
1	A	10	LYS	N-CA	6.94	1.55	1.46
1	A	212	GLY	CA-C	6.91	1.59	1.52
1	A	124	GLU	CA-C	-6.90	1.43	1.52
1	A	219	GLN	C-O	-6.88	1.15	1.24
1	A	82	ASP	CA-C	6.87	1.61	1.53
1	A	146	ASP	CA-C	6.84	1.61	1.52
1	A	143	ASN	N-CA	6.82	1.55	1.46
1	A	86	ILE	CA-CB	6.80	1.64	1.54
1	A	248	PHE	C-N	-6.75	1.24	1.33
1	A	124	GLU	N-CA	6.73	1.54	1.46
1	A	272	ALA	C-N	-6.73	1.23	1.34
1	A	154	GLY	N-CA	6.70	1.54	1.45
1	A	116	ARG	N-CA	6.69	1.54	1.46
1	A	141	THR	CA-C	-6.69	1.44	1.52
1	A	76	ALA	CA-C	-6.68	1.44	1.52
1	A	266	MET	SD-CE	-6.67	1.62	1.79
1	A	251	SER	C-O	6.65	1.31	1.23
1	A	63	ILE	CA-C	-6.62	1.44	1.52
1	A	280	PHE	C-O	6.62	1.31	1.23
1	A	258	VAL	CA-C	6.55	1.60	1.52
1	A	291	ARG	C-N	-6.48	1.25	1.33
1	A	299	GLU	C-N	-6.47	1.25	1.34
1	A	47	LEU	N-CA	6.46	1.54	1.46
1	A	73	ALA	C-N	6.44	1.42	1.33
1	A	77	LYS	C-N	6.44	1.42	1.33
1	A	254	PRO	CA-CB	6.44	1.62	1.53
1	A	100	MET	C-N	-6.42	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	LEU	N-CA	-6.39	1.38	1.46
1	A	152	THR	N-CA	6.39	1.54	1.46
1	A	160	LYS	C-N	-6.28	1.25	1.33
1	A	67	ASP	C-N	-6.22	1.24	1.33
1	A	185	ALA	N-CA	-6.20	1.39	1.46
1	A	259	HIS	CG-ND1	6.18	1.45	1.38
1	A	31	LEU	C-N	-6.17	1.24	1.33
1	A	104	PRO	CA-CB	-6.17	1.45	1.53
1	A	184	ASP	N-CA	6.16	1.53	1.46
1	A	137	VAL	C-O	6.11	1.31	1.24
1	A	232	ASN	CG-OD1	6.10	1.35	1.23
1	A	241	SER	N-CA	-6.09	1.38	1.46
1	A	180	PRO	C-N	-6.02	1.26	1.33
1	A	188	SER	C-N	-6.00	1.25	1.33
1	A	138	MET	CA-CB	-5.97	1.44	1.53
1	A	203	GLY	CA-C	5.96	1.56	1.51
1	A	279	LYS	N-CA	-5.96	1.38	1.46
1	A	110	ALA	C-O	5.96	1.31	1.24
1	A	182	ALA	CA-C	-5.95	1.45	1.52
1	A	16	TRP	C-O	5.93	1.30	1.24
1	A	262	LYS	CA-CB	-5.91	1.43	1.53
1	A	50	ILE	N-CA	5.90	1.53	1.46
1	A	215	ALA	C-N	5.90	1.41	1.33
1	A	202	VAL	CA-CB	-5.86	1.47	1.54
1	A	173	PRO	CA-C	-5.82	1.45	1.52
1	A	197	LYS	N-CA	5.78	1.53	1.46
1	A	12	PRO	C-N	-5.77	1.25	1.33
1	A	231	ILE	CA-C	-5.77	1.45	1.52
1	A	194	PRO	N-CD	5.76	1.55	1.47
1	A	263	SER	C-O	5.73	1.30	1.24
1	A	79	ARG	NE-CZ	5.73	1.39	1.33
1	A	134	GLU	CA-CB	-5.72	1.45	1.53
1	A	87	ALA	CA-C	5.72	1.60	1.52
1	A	227	ILE	C-N	-5.70	1.25	1.33
1	A	130	TRP	C-N	-5.68	1.25	1.33
1	A	116	ARG	CA-C	-5.68	1.45	1.52
1	A	297	GLU	C-N	-5.67	1.26	1.34
1	A	42	ASP	C-N	-5.64	1.25	1.33
1	A	239	GLU	C-N	-5.64	1.26	1.33
1	A	17	PHE	CA-CB	5.63	1.62	1.53
1	A	140	ILE	N-CA	5.63	1.52	1.46
1	A	126	GLN	N-CA	5.62	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	PRO	C-O	5.61	1.31	1.24
1	A	171	GLN	C-N	-5.61	1.27	1.33
1	A	257	ASP	N-CA	-5.59	1.39	1.46
1	A	8	LEU	CA-CB	5.59	1.61	1.53
1	A	58	ALA	C-N	5.59	1.41	1.33
1	A	44	GLU	CA-CB	5.58	1.62	1.53
1	A	274	ASP	C-O	5.56	1.30	1.24
1	A	111	THR	C-O	-5.54	1.17	1.24
1	A	269	ASN	CB-CG	5.54	1.66	1.52
1	A	243	ALA	CA-C	-5.52	1.45	1.52
1	A	149	ARG	CZ-NH2	5.51	1.40	1.33
1	A	279	LYS	C-O	-5.50	1.17	1.24
1	A	191	VAL	N-CA	5.49	1.53	1.46
1	A	291	ARG	CA-C	5.49	1.60	1.52
1	A	216	THR	CA-CB	5.48	1.61	1.53
1	A	65	THR	C-N	5.46	1.40	1.34
1	A	110	ALA	CA-C	-5.45	1.45	1.52
1	A	22	LYS	N-CA	5.44	1.52	1.46
1	A	44	GLU	C-N	5.43	1.41	1.33
1	A	165	PRO	C-N	-5.40	1.26	1.33
1	A	150	ARG	CA-C	5.38	1.60	1.52
1	A	136	ALA	C-O	5.36	1.30	1.23
1	A	200	LEU	C-O	5.35	1.30	1.24
1	A	259	HIS	CA-C	-5.34	1.46	1.52
1	A	147	THR	C-N	-5.33	1.26	1.33
1	A	300	LYS	C-O	5.33	1.30	1.24
1	A	282	GLU	C-N	-5.32	1.25	1.33
1	A	268	TYR	C-O	5.27	1.30	1.24
1	A	246	THR	CA-C	-5.27	1.45	1.52
1	A	137	VAL	N-CA	-5.25	1.39	1.46
1	A	237	VAL	C-O	5.25	1.30	1.24
1	A	106	VAL	N-CA	5.25	1.52	1.46
1	A	20	GLU	CA-C	-5.23	1.46	1.52
1	A	47	LEU	CA-C	-5.23	1.46	1.52
1	A	113	ILE	C-N	5.23	1.40	1.33
1	A	185	ALA	C-N	5.23	1.40	1.33
1	A	98	LYS	N-CA	-5.22	1.38	1.46
1	A	246	THR	C-O	5.21	1.31	1.23
1	A	173	PRO	N-CD	5.19	1.55	1.47
1	A	93	VAL	CA-C	5.19	1.58	1.52
1	A	103	VAL	C-N	-5.18	1.26	1.33
1	A	34	GLU	CA-CB	-5.18	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	VAL	C-N	-5.17	1.26	1.33
1	A	250	GLY	C-O	5.17	1.30	1.23
1	A	268	TYR	C-N	-5.17	1.27	1.33
1	A	109	ALA	C-O	5.15	1.29	1.23
1	A	218	GLY	C-O	5.15	1.30	1.24
1	A	127	LYS	C-N	5.14	1.41	1.33
1	A	46	THR	C-N	5.14	1.41	1.33
1	A	72	SER	C-N	5.14	1.41	1.33
1	A	208	THR	CA-C	-5.12	1.46	1.52
1	A	139	ALA	C-O	5.12	1.30	1.24
1	A	66	PRO	N-CA	-5.10	1.40	1.47
1	A	232	ASN	CA-C	5.08	1.59	1.52
1	A	72	SER	CA-CB	5.08	1.61	1.53
1	A	277	PRO	CA-CB	5.06	1.60	1.54
1	A	22	LYS	C-O	5.05	1.30	1.24
1	A	131	ASP	C-N	-5.04	1.27	1.34
1	A	281	THR	C-O	5.04	1.29	1.24
1	A	33	PHE	N-CA	5.04	1.52	1.45
1	A	260	GLY	C-N	5.01	1.41	1.33
1	A	122	TYR	C-N	-5.01	1.27	1.33

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ASN	OD1-CG-ND2	12.56	135.16	122.60
1	A	143	ASN	OD1-CG-ND2	-12.45	110.15	122.60
1	A	201	ILE	CB-CG1-CD1	12.20	139.42	113.80
1	A	103	VAL	O-C-N	12.17	130.95	121.46
1	A	285	ASP	CA-CB-CG	11.53	124.13	112.60
1	A	237	VAL	CA-C-O	-11.40	109.09	120.95
1	A	291	ARG	NE-CZ-NH1	11.39	132.89	121.50
1	A	146	ASP	O-C-N	11.11	133.64	122.09
1	A	150	ARG	NE-CZ-NH2	-10.75	109.53	119.20
1	A	188	SER	O-C-N	-10.69	110.79	122.12
1	A	92	PHE	CA-CB-CG	10.43	124.23	113.80
1	A	274	ASP	CA-CB-CG	-10.42	102.18	112.60
1	A	116	ARG	NE-CZ-NH1	10.27	131.77	121.50
1	A	79	ARG	NE-CZ-NH1	10.23	131.73	121.50
1	A	131	ASP	CA-CB-CG	9.93	122.53	112.60
1	A	79	ARG	CG-CD-NE	9.66	133.24	112.00
1	A	49	ALA	CA-C-O	-9.64	109.21	120.10
1	A	131	ASP	CA-C-O	-9.60	109.35	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	HIS	CA-CB-CG	-9.55	104.25	113.80
1	A	111	THR	O-C-N	9.38	132.06	122.12
1	A	300	LYS	N-CA-CB	9.22	124.42	110.22
1	A	256	PRO	O-C-N	-9.16	109.96	122.24
1	A	300	LYS	CA-CB-CG	9.07	132.25	114.10
1	A	18	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	A	231	ILE	CA-C-N	8.95	138.64	121.54
1	A	231	ILE	C-N-CA	8.95	138.64	121.54
1	A	213	VAL	O-C-N	8.94	131.20	121.90
1	A	110	ALA	O-C-N	-8.83	112.76	122.12
1	A	202	VAL	CA-C-O	-8.79	111.16	120.48
1	A	256	PRO	CA-C-O	8.73	131.66	119.18
1	A	74	ILE	CA-C-O	-8.64	112.01	121.17
1	A	286	VAL	CA-C-O	-8.60	112.88	120.96
1	A	74	ILE	O-C-N	8.52	130.26	121.91
1	A	296	GLU	CB-CA-C	-8.51	96.39	110.85
1	A	183	PHE	CA-C-O	8.47	129.72	120.82
1	A	141	THR	CA-CB-OG1	-8.45	96.93	109.60
1	A	139	ALA	CA-C-O	-8.44	111.43	120.46
1	A	99	PRO	CA-C-O	-8.44	112.12	121.32
1	A	260	GLY	O-C-N	-8.34	114.18	122.18
1	A	297	GLU	CA-C-O	-8.33	111.59	120.42
1	A	299	GLU	CA-C-O	-8.31	111.61	120.42
1	A	77	LYS	CA-CB-CG	8.25	130.61	114.10
1	A	103	VAL	CA-C-O	-8.19	113.22	119.20
1	A	302	GLY	CA-C-O	8.18	128.22	119.06
1	A	251	SER	CA-C-N	8.08	133.17	122.42
1	A	251	SER	C-N-CA	8.08	133.17	122.42
1	A	150	ARG	CA-CB-CG	-7.97	98.17	114.10
1	A	291	ARG	O-C-N	7.96	131.54	122.22
1	A	144	GLU	CB-CG-CD	7.93	126.09	112.60
1	A	169	ILE	CA-C-O	-7.91	111.57	120.74
1	A	26	LYS	O-C-N	7.85	130.15	122.07
1	A	222	LYS	CA-C-N	7.83	131.10	120.38
1	A	222	LYS	C-N-CA	7.83	131.10	120.38
1	A	215	ALA	CA-C-O	7.73	128.74	120.55
1	A	215	ALA	O-C-N	-7.70	113.96	122.12
1	A	149	ARG	NH1-CZ-NH2	7.66	129.26	119.30
1	A	22	LYS	CG-CD-CE	-7.64	93.72	111.30
1	A	164	PHE	CA-CB-CG	-7.62	106.18	113.80
1	A	213	VAL	CA-C-O	-7.62	112.59	121.05
1	A	80	GLY	CA-C-O	7.59	128.60	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	LEU	CA-C-O	7.58	128.69	120.58
1	A	294	PHE	CA-CB-CG	7.57	121.37	113.80
1	A	288	LEU	O-C-N	-7.51	113.78	123.02
1	A	88	VAL	CA-C-N	7.50	135.87	121.54
1	A	88	VAL	C-N-CA	7.50	135.87	121.54
1	A	116	ARG	NH1-CZ-NH2	-7.46	109.60	119.30
1	A	200	LEU	CA-C-O	-7.46	112.11	120.54
1	A	145	LEU	O-C-N	-7.42	114.76	123.22
1	A	79	ARG	NH1-CZ-NH2	-7.41	109.67	119.30
1	A	296	GLU	N-CA-CB	7.40	121.12	110.16
1	A	86	ILE	O-C-N	-7.39	115.19	123.10
1	A	37	LYS	CG-CD-CE	7.38	128.26	111.30
1	A	191	VAL	CA-C-O	-7.36	109.89	119.53
1	A	302	GLY	O-C-N	-7.30	113.15	122.43
1	A	267	LEU	CA-C-O	7.29	128.48	120.82
1	A	222	LYS	O-C-N	-7.26	114.81	122.94
1	A	79	ARG	CA-CB-CG	7.25	128.59	114.10
1	A	241	SER	CA-CB-OG	-7.22	96.66	111.10
1	A	12	PRO	N-CD-CG	-7.22	92.37	103.20
1	A	274	ASP	CA-C-O	7.20	130.81	120.51
1	A	249	TYR	CB-CG-CD1	-7.17	110.04	120.80
1	A	101	ASP	CA-CB-CG	-7.17	105.43	112.60
1	A	188	SER	CA-C-N	7.16	130.46	120.29
1	A	188	SER	C-N-CA	7.16	130.46	120.29
1	A	124	GLU	O-C-N	-7.15	114.00	122.15
1	A	274	ASP	O-C-N	-7.11	113.13	122.59
1	A	23	PHE	CA-CB-CG	-7.09	106.71	113.80
1	A	283	VAL	CB-CA-C	7.06	120.44	110.84
1	A	141	THR	CA-CB-CG2	7.05	122.48	110.50
1	A	38	ILE	CA-C-N	7.01	131.53	121.50
1	A	38	ILE	C-N-CA	7.01	131.53	121.50
1	A	26	LYS	CA-C-O	-6.99	113.48	120.82
1	A	60	GLY	N-CA-C	-6.98	100.02	110.42
1	A	117	GLN	O-C-N	-6.95	114.91	122.07
1	A	263	SER	CA-C-N	6.89	129.52	120.28
1	A	263	SER	C-N-CA	6.89	129.52	120.28
1	A	100	MET	O-C-N	-6.88	114.12	122.71
1	A	43	GLY	O-C-N	-6.87	115.50	122.17
1	A	109	ALA	CA-C-O	-6.85	114.08	122.36
1	A	143	ASN	N-CA-C	6.83	120.72	112.38
1	A	141	THR	CA-C-N	6.82	132.69	122.87
1	A	141	THR	C-N-CA	6.82	132.69	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ALA	O-C-N	6.82	131.78	122.37
1	A	64	CYS	N-CA-CB	6.79	121.93	110.46
1	A	87	ALA	CA-C-O	-6.77	113.14	120.92
1	A	142	ALA	N-CA-C	-6.77	100.27	109.54
1	A	138	MET	CB-CG-SD	-6.75	92.45	112.70
1	A	100	MET	CA-C-N	6.75	134.42	121.54
1	A	100	MET	C-N-CA	6.75	134.42	121.54
1	A	259	HIS	CA-C-O	-6.73	113.75	120.82
1	A	4	LYS	CA-CB-CG	-6.71	100.68	114.10
1	A	168	GLN	N-CA-C	-6.63	104.50	112.59
1	A	136	ALA	O-C-N	-6.63	116.33	123.42
1	A	87	ALA	O-C-N	6.60	130.82	123.16
1	A	147	THR	CA-CB-OG1	-6.57	99.75	109.60
1	A	38	ILE	O-C-N	-6.55	116.12	123.20
1	A	60	GLY	O-C-N	6.52	131.18	123.61
1	A	120	GLU	OE1-CD-OE2	6.47	138.44	122.90
1	A	291	ARG	NE-CZ-NH2	-6.47	113.38	119.20
1	A	290	THR	CA-CB-CG2	6.43	121.43	110.50
1	A	130	TRP	CB-CG-CD2	-6.40	117.84	126.80
1	A	97	GLY	CA-C-N	6.39	133.08	120.94
1	A	97	GLY	C-N-CA	6.39	133.08	120.94
1	A	87	ALA	CA-C-N	-6.37	114.27	123.06
1	A	87	ALA	C-N-CA	-6.37	114.27	123.06
1	A	263	SER	CA-C-O	-6.33	113.85	120.55
1	A	217	GLU	CG-CD-OE1	6.30	132.90	118.40
1	A	24	ALA	N-CA-C	-6.30	104.49	111.36
1	A	103	VAL	CA-CB-CG1	6.30	121.11	110.40
1	A	51	ASP	CA-C-N	6.29	128.61	120.44
1	A	51	ASP	C-N-CA	6.29	128.61	120.44
1	A	120	GLU	CG-CD-OE2	-6.27	103.97	118.40
1	A	144	GLU	CG-CD-OE1	6.27	132.82	118.40
1	A	192	GLN	CA-C-N	-6.26	115.26	123.34
1	A	192	GLN	C-N-CA	-6.26	115.26	123.34
1	A	249	TYR	CD1-CG-CD2	6.23	127.45	118.10
1	A	106	VAL	O-C-N	-6.23	115.81	123.10
1	A	281	THR	CA-C-O	-6.20	113.89	120.40
1	A	166	GLU	O-C-N	-6.18	115.57	122.12
1	A	292	ASP	CB-CG-OD2	-6.17	104.20	118.40
1	A	244	GLN	OE1-CD-NE2	6.15	128.75	122.60
1	A	140	ILE	CB-CA-C	6.12	117.84	111.23
1	A	248	PHE	CA-C-O	-6.12	114.37	120.98
1	A	253	LEU	CA-C-N	6.09	127.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	LEU	C-N-CA	6.09	127.45	119.84
1	A	29	LYS	N-CA-CB	6.08	118.83	110.01
1	A	290	THR	CA-CB-OG1	-6.05	100.52	109.60
1	A	291	ARG	CA-C-O	-6.05	113.26	120.10
1	A	110	ALA	N-CA-C	6.04	118.64	111.33
1	A	67	ASP	CA-C-O	-6.03	111.89	120.16
1	A	223	ALA	CA-C-O	-6.03	114.11	120.63
1	A	96	LYS	O-C-N	-6.02	112.78	122.41
1	A	300	LYS	CA-C-O	-6.01	113.30	120.10
1	A	296	GLU	CG-CD-OE2	-6.00	104.60	118.40
1	A	131	ASP	O-C-N	5.93	130.32	123.02
1	A	216	THR	CA-CB-OG1	-5.93	100.71	109.60
1	A	299	GLU	O-C-N	5.92	128.90	122.15
1	A	171	GLN	OE1-CD-NE2	5.90	128.50	122.60
1	A	145	LEU	CA-C-O	5.88	126.65	120.36
1	A	214	ARG	CD-NE-CZ	-5.87	116.18	124.40
1	A	140	ILE	O-C-N	-5.87	116.28	122.68
1	A	31	LEU	CA-C-O	-5.86	112.21	119.18
1	A	42	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	240	LEU	CA-C-N	5.84	132.97	121.58
1	A	240	LEU	C-N-CA	5.84	132.97	121.58
1	A	114	GLY	O-C-N	5.83	127.84	122.19
1	A	281	THR	CA-C-N	5.81	130.50	122.77
1	A	281	THR	C-N-CA	5.81	130.50	122.77
1	A	139	ALA	CA-C-N	5.81	130.26	122.01
1	A	139	ALA	C-N-CA	5.81	130.26	122.01
1	A	242	LYS	CA-C-O	-5.81	115.39	121.55
1	A	249	TYR	O-C-N	-5.81	114.68	122.23
1	A	42	ASP	CA-C-N	5.81	126.53	120.03
1	A	42	ASP	C-N-CA	5.81	126.53	120.03
1	A	191	VAL	O-C-N	5.81	130.21	122.31
1	A	65	THR	N-CA-C	5.80	117.19	109.83
1	A	22	LYS	CB-CG-CD	-5.79	97.99	111.30
1	A	266	MET	N-CA-C	-5.78	104.97	111.28
1	A	149	ARG	CA-CB-CG	-5.78	102.54	114.10
1	A	128	ARG	CA-CB-CG	-5.73	102.64	114.10
1	A	79	ARG	CA-C-N	5.73	127.30	120.14
1	A	79	ARG	C-N-CA	5.73	127.30	120.14
1	A	166	GLU	CA-C-O	5.70	126.79	120.63
1	A	124	GLU	N-CA-C	-5.70	105.15	111.36
1	A	260	GLY	CA-C-O	5.70	127.15	121.00
1	A	67	ASP	CB-CG-OD1	5.69	131.48	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	CA-C-N	5.69	128.16	120.65
1	A	75	VAL	C-N-CA	5.69	128.16	120.65
1	A	102	THR	N-CA-C	5.69	120.22	113.28
1	A	116	ARG	CG-CD-NE	-5.68	99.51	112.00
1	A	278	PRO	CA-C-N	5.66	128.92	120.31
1	A	278	PRO	C-N-CA	5.66	128.92	120.31
1	A	155	SER	O-C-N	-5.66	115.98	122.09
1	A	289	ILE	CA-C-O	5.66	127.17	120.72
1	A	151	ARG	NH1-CZ-NH2	-5.65	111.96	119.30
1	A	99	PRO	N-CD-CG	-5.64	94.73	103.20
1	A	72	SER	N-CA-C	5.64	117.43	111.28
1	A	251	SER	O-C-N	-5.64	116.95	123.33
1	A	150	ARG	CD-NE-CZ	5.64	132.29	124.40
1	A	130	TRP	CB-CG-CD1	5.62	135.34	126.90
1	A	291	ARG	CB-CA-C	-5.61	100.25	110.63
1	A	80	GLY	CA-C-N	-5.60	113.69	122.65
1	A	80	GLY	C-N-CA	-5.60	113.69	122.65
1	A	177	ASN	N-CA-CB	-5.59	103.70	110.53
1	A	249	TYR	CG-CD1-CE1	-5.59	112.81	121.20
1	A	244	GLN	N-CA-C	5.59	119.21	110.32
1	A	271	VAL	N-CA-CB	-5.54	102.27	110.58
1	A	52	SER	CA-C-N	5.53	127.69	120.28
1	A	52	SER	C-N-CA	5.53	127.69	120.28
1	A	301	LYS	O-C-N	-5.53	115.26	122.39
1	A	56	SER	CA-C-O	-5.51	112.62	119.18
1	A	29	LYS	CB-CA-C	-5.50	102.25	110.88
1	A	119	GLN	CG-CD-OE1	5.49	131.78	120.80
1	A	276	GLU	CA-C-O	5.49	124.92	119.49
1	A	161	ALA	N-CA-C	-5.49	105.38	111.36
1	A	192	GLN	CA-CB-CG	-5.48	103.13	114.10
1	A	149	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	A	62	VAL	N-CA-CB	5.47	119.61	110.86
1	A	151	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	163	GLY	CA-C-O	-5.44	113.51	118.95
1	A	221	PHE	CA-C-O	-5.44	114.67	120.92
1	A	61	PHE	CD1-CG-CD2	5.43	126.75	118.60
1	A	292	ASP	CA-C-O	-5.42	114.68	120.42
1	A	205	ASN	O-C-N	5.40	129.23	122.92
1	A	259	HIS	CA-C-N	5.39	125.93	119.94
1	A	259	HIS	C-N-CA	5.39	125.93	119.94
1	A	146	ASP	CA-C-O	-5.39	115.14	120.90
1	A	42	ASP	CA-C-O	-5.38	115.70	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	VAL	O-C-N	5.37	127.08	121.87
1	A	53	LEU	O-C-N	5.36	127.80	122.12
1	A	282	GLU	CG-CD-OE1	-5.35	106.10	118.40
1	A	193	HIS	CA-C-N	5.33	125.00	119.56
1	A	193	HIS	C-N-CA	5.33	125.00	119.56
1	A	94	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	268	TYR	CA-C-O	-5.32	115.24	120.82
1	A	211	GLY	O-C-N	-5.30	117.10	122.19
1	A	235	ASP	CB-CG-OD1	5.30	130.60	118.40
1	A	148	ALA	CA-C-O	5.29	126.15	120.70
1	A	109	ALA	CA-C-N	5.25	127.57	120.38
1	A	109	ALA	C-N-CA	5.25	127.57	120.38
1	A	283	VAL	CA-CB-CG2	5.25	119.32	110.40
1	A	256	PRO	CA-C-N	5.23	127.55	120.44
1	A	256	PRO	C-N-CA	5.23	127.55	120.44
1	A	136	ALA	CA-C-N	5.22	129.51	122.93
1	A	136	ALA	C-N-CA	5.22	129.51	122.93
1	A	232	ASN	CA-C-O	-5.22	113.04	120.51
1	A	133	LYS	CA-C-N	-5.22	114.28	122.79
1	A	133	LYS	C-N-CA	-5.22	114.28	122.79
1	A	63	ILE	N-CA-C	5.22	115.24	108.35
1	A	247	GLY	O-C-N	-5.21	116.80	122.84
1	A	232	ASN	O-C-N	5.21	129.51	122.59
1	A	27	ALA	O-C-N	-5.20	116.61	122.12
1	A	27	ALA	CA-C-O	5.20	126.24	120.63
1	A	254	PRO	N-CA-CB	5.18	108.69	103.25
1	A	135	SER	CA-C-O	-5.17	115.42	121.46
1	A	249	TYR	N-CA-CB	-5.16	102.50	110.20
1	A	296	GLU	CB-CG-CD	-5.16	103.82	112.60
1	A	296	GLU	O-C-N	5.16	128.03	122.15
1	A	269	ASN	CB-CG-OD1	-5.16	110.48	120.80
1	A	127	LYS	CG-CD-CE	-5.16	99.44	111.30
1	A	167	LYS	CA-CB-CG	-5.15	103.80	114.10
1	A	153	THR	CA-C-O	-5.14	115.41	120.70
1	A	225	ASP	CA-CB-CG	-5.14	107.46	112.60
1	A	44	GLU	CA-CB-CG	-5.13	103.83	114.10
1	A	111	THR	CA-C-O	-5.13	115.11	120.55
1	A	117	GLN	CG-CD-OE1	-5.13	110.53	120.80
1	A	164	PHE	CA-C-N	5.13	126.26	119.84
1	A	164	PHE	C-N-CA	5.13	126.26	119.84
1	A	138	MET	N-CA-CB	5.13	118.99	110.47
1	A	278	PRO	O-C-N	-5.12	116.71	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ASN	CA-C-O	-5.11	116.04	122.63
1	A	117	GLN	CG-CD-NE2	5.10	124.05	116.40
1	A	67	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	200	LEU	N-CA-CB	5.08	118.54	110.16
1	A	98	LYS	CB-CA-C	-5.08	101.18	109.41
1	A	72	SER	CA-C-O	5.07	125.92	120.55
1	A	119	GLN	N-CA-C	-5.07	105.65	111.07
1	A	263	SER	CB-CA-C	5.06	119.18	110.79
1	A	252	LEU	O-C-N	-5.05	116.86	122.93
1	A	209	VAL	CA-C-O	-5.05	115.49	120.85
1	A	76	ALA	CA-C-O	-5.04	115.70	121.00
1	A	262	LYS	CA-C-N	-5.04	113.53	120.28
1	A	262	LYS	C-N-CA	-5.04	113.53	120.28
1	A	143	ASN	CB-CG-OD1	5.04	130.88	120.80
1	A	288	LEU	CA-C-N	5.03	129.59	123.10
1	A	288	LEU	C-N-CA	5.03	129.59	123.10
1	A	11	GLN	CA-C-N	5.01	124.67	119.56
1	A	11	GLN	C-N-CA	5.01	124.67	119.56
1	A	138	MET	N-CA-C	-5.01	99.12	107.99

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	2315	0	2324	44	3
2	A	11	0	12	0	0
3	A	11	0	11	1	0
4	A	191	0	0	17	4
All	All	2528	0	2347	44	4

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 (44) 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:741:HOH:O	1.37	1.24
1:A:295:LYS:HD2	4:A:757:HOH:O	1.58	1.04
1:A:69:LYS:NZ	4:A:726:HOH:O	1.99	0.95
1:A:294:PHE:HE1	4:A:756:HOH:O	1.61	0.82
1:A:296:GLU:HG3	4:A:433:HOH:O	1.84	0.76
1:A:109:ALA:O	1:A:113:ILE:HD12	1.87	0.75
1:A:274:ASP:OD2	4:A:764:HOH:O	2.05	0.74
1:A:160:LYS:HD3	1:A:166:GLU:CG	2.19	0.72
1:A:160:LYS:HD3	1:A:166:GLU:HG3	1.73	0.71
1:A:106:VAL:CG2	1:A:266:MET:HE1	2.24	0.68
1:A:175:LYS:HD2	4:A:441:HOH:O	1.94	0.66
1:A:75:VAL:O	1:A:79:ARG:HG2	1.95	0.65
1:A:143:ASN:OD1	1:A:149:ARG:HG3	1.97	0.65
1:A:146:ASP:CB	4:A:741:HOH:O	2.13	0.62
1:A:274:ASP:CG	4:A:764:HOH:O	2.44	0.60
1:A:146:ASP:CG	4:A:741:HOH:O	2.38	0.60
1:A:106:VAL:HG21	1:A:266:MET:HE1	1.84	0.60
1:A:296:GLU:CD	4:A:569:HOH:O	2.46	0.58
1:A:99:PRO:HG3	4:A:739:HOH:O	2.06	0.56
1:A:257:ASP:OD2	1:A:301:LYS:NZ	2.35	0.56
1:A:270:TRP:NE1	1:A:276:GLU:OE1	2.41	0.54
1:A:269:ASN:ND2	4:A:507:HOH:O	1.87	0.52
1:A:26:LYS:HA	1:A:29:LYS:HD2	1.90	0.52
1:A:255:SER:OG	1:A:301:LYS:HE3	2.10	0.52
1:A:171:GLN:HG3	4:A:450:HOH:O	2.12	0.50
1:A:273:LYS:O	1:A:274:ASP:C	2.54	0.49
1:A:122:TYR:CE1	1:A:125:MET:CE	2.96	0.49
1:A:160:LYS:HD3	1:A:166:GLU:HG2	1.93	0.49
1:A:172:VAL:HB	1:A:189:MET:HE3	1.95	0.48
1:A:112:LYS:HD3	1:A:112:LYS:HA	1.54	0.48
1:A:68:PRO:HB3	1:A:91:GLN:O	2.15	0.47
1:A:295:LYS:CD	4:A:757:HOH:O	2.37	0.47
1:A:122:TYR:CE1	1:A:125:MET:HE1	2.50	0.47
1:A:212:GLY:O	1:A:216:THR:HG23	2.15	0.46
1:A:188:SER:HB3	4:A:608:HOH:O	2.15	0.45
1:A:276:GLU:HA	1:A:277:PRO:HD3	1.85	0.44
1:A:286:VAL:HG22	1:A:287:VAL:N	2.33	0.43
1:A:103:VAL:HG22	4:A:781:HOH:O	2.18	0.43
1:A:160:LYS:CD	1:A:166:GLU:HG3	2.46	0.42
1:A:297:GLU:CD	1:A:300:LYS:HE3	2.45	0.41
1:A:179:ILE:N	1:A:180:PRO:CD	2.83	0.41
1:A:16:TRP:CZ2	3:A:308[B]:FCB:H63	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:HA	1:A:99:PRO:HD3	1.82	0.41
1:A:134:GLU:H	1:A:134:GLU:HG2	1.74	0.40

All (4) 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:495:HOH:O	4:A:774:HOH:O[4_466]	1.62	0.58
1:A:262:LYS:NZ	4:A:591:HOH:O[4_566]	1.90	0.30
1:A:295:LYS:CG	4:A:656:HOH:O[4_466]	1.90	0.30
1:A:295:LYS:CB	4:A:656:HOH:O[4_466]	1.98	0.22

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	295 (97%)	5 (2%)	3 (1%)	12 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	101	ASP
1	A	254	PRO

5.3.2 Protein sidechains [i](#)

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%)	225 (93%)	18 (7%)	13 6

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PRO
1	A	22	LYS
1	A	37	LYS
1	A	59	LYS
1	A	72	SER
1	A	79	ARG
1	A	98	LYS
1	A	99	PRO
1	A	108	MET
1	A	113	ILE
1	A	123	LYS
1	A	127	LYS
1	A	144	GLU
1	A	167	LYS
1	A	175	LYS
1	A	201	ILE
1	A	204	MET
1	A	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
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	1.52	2 (18%)	16,16,16	1.00	0
3	FCB	A	308[B]	-	11,11,11	2.51	3 (27%)	16,16,16	1.38	4 (25%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	308[B]	FCB	C3-C2	-6.08	1.36	1.52
3	A	308[B]	FCB	O3-C3	4.65	1.54	1.43
2	A	307[A]	FCA	O2-C2	3.22	1.50	1.43
2	A	307[A]	FCA	O5-C1	2.94	1.50	1.42
3	A	308[B]	FCB	C4-C3	2.02	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	308[B]	FCB	C3-C4-C5	-3.11	105.08	109.81
3	A	308[B]	FCB	O3-C3-C4	-2.12	105.37	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	308[B]	FCB	C1-O5-C5	2.06	117.58	114.37
3	A	308[B]	FCB	C4-C3-C2	2.05	114.43	110.83

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]	FCB	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.