



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:20 PM GMT

PDB ID : 1ABF  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

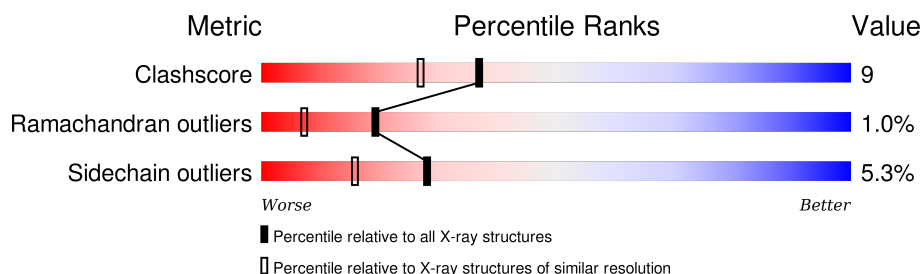
# 1 Overall quality at a glance

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	

## 2 Entry composition [i](#)

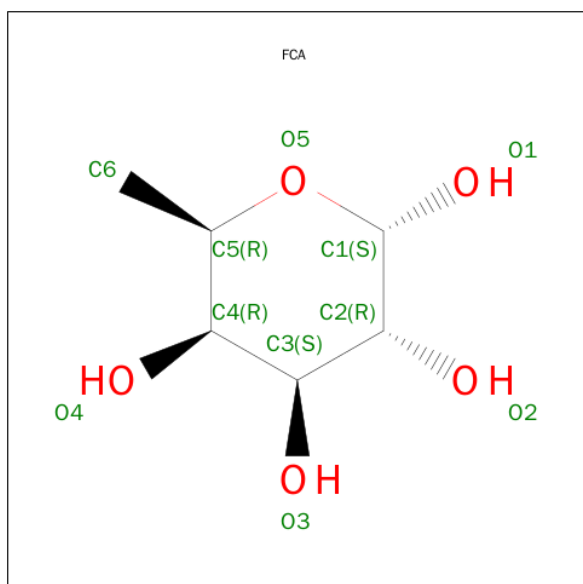
There are 4 unique types of molecules in this entry. The entry contains 2528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

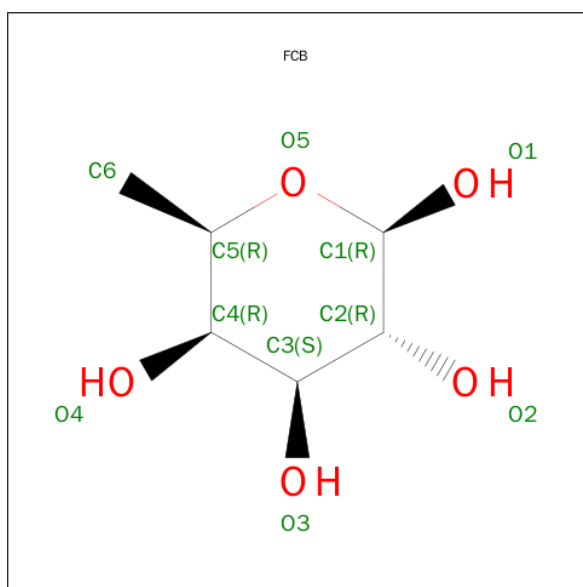
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2315	1473	388	443	11	0	0	0

- Molecule 2 is SUGAR (2-MER) (three-letter code: FCA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



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

- Molecule 3 is water (three-letter code: FCB) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



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

- Molecule 4 is water.

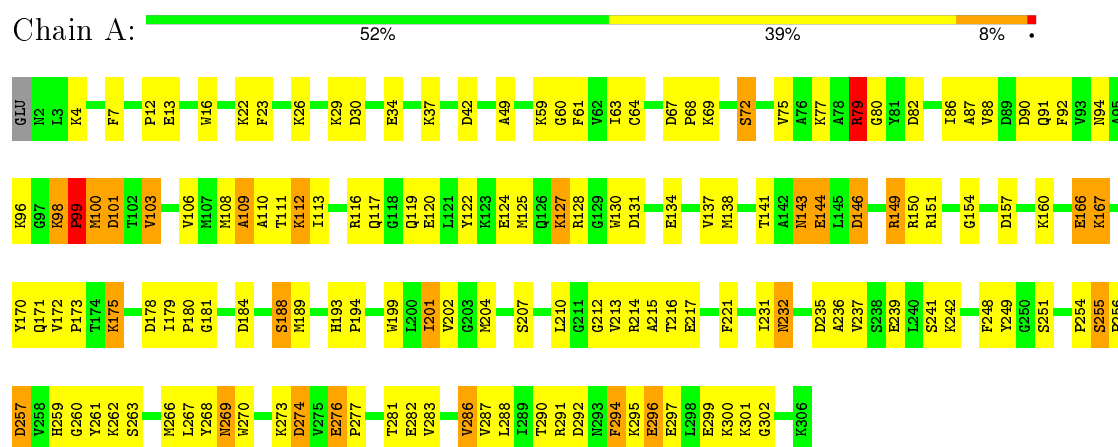
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total	O	0	0
			191	191		

### 3 Residue-property plots

These plots are drawn for all protein, RNA 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	17.0	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: 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	2.08	48/2360 (2.0%)	2.57	141/3188 (4.4%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	ARG	NE-CZ	8.37	1.44	1.33
1	A	120	GLU	CD-OE2	-8.28	1.16	1.25
1	A	124	GLU	CD-OE1	-7.75	1.17	1.25
1	A	120	GLU	CD-OE1	-6.81	1.18	1.25
1	A	60	GLY	N-CA	6.78	1.56	1.46
1	A	221	PHE	CE2-CZ	6.75	1.50	1.37
1	A	120	GLU	CG-CD	6.72	1.62	1.51
1	A	267	LEU	N-CA	6.52	1.59	1.46
1	A	269	ASN	CB-CG	6.46	1.66	1.51
1	A	297	GLU	C-O	6.34	1.35	1.23
1	A	207	SER	CB-OG	-6.28	1.34	1.42
1	A	116	ARG	CD-NE	6.26	1.57	1.46
1	A	259	HIS	N-CA	6.17	1.58	1.46
1	A	88	VAL	C-O	6.16	1.35	1.23
1	A	297	GLU	CD-OE2	-6.10	1.19	1.25
1	A	144	GLU	CD-OE2	6.07	1.32	1.25
1	A	181	GLY	CA-C	-5.99	1.42	1.51
1	A	88	VAL	CB-CG2	5.97	1.65	1.52
1	A	80	GLY	CA-C	-5.88	1.42	1.51
1	A	13	GLU	CD-OE1	-5.85	1.19	1.25
1	A	221	PHE	CG-CD1	5.84	1.47	1.38
1	A	149	ARG	CZ-NH2	5.82	1.40	1.33
1	A	92	PHE	CG-CD1	5.79	1.47	1.38
1	A	188	SER	CB-OG	5.78	1.49	1.42
1	A	255	SER	CB-OG	5.74	1.49	1.42
1	A	63	ILE	CA-CB	5.73	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	ALA	N-CA	-5.72	1.34	1.46
1	A	61	PHE	CB-CG	5.71	1.61	1.51
1	A	194	PRO	N-CD	5.69	1.55	1.47
1	A	251	SER	CB-OG	5.65	1.49	1.42
1	A	154	GLY	N-CA	5.60	1.54	1.46
1	A	202	VAL	C-N	-5.53	1.23	1.33
1	A	86	ILE	C-O	5.53	1.33	1.23
1	A	249	TYR	CE1-CZ	-5.53	1.31	1.38
1	A	72	SER	CA-CB	5.51	1.61	1.52
1	A	261	TYR	CG-CD2	-5.43	1.32	1.39
1	A	82	ASP	CB-CG	5.35	1.62	1.51
1	A	94	ASN	N-CA	5.33	1.57	1.46
1	A	23	PHE	CB-CG	5.33	1.60	1.51
1	A	194	PRO	N-CA	-5.30	1.38	1.47
1	A	37	LYS	CD-CE	-5.29	1.38	1.51
1	A	263	SER	N-CA	5.29	1.56	1.46
1	A	7	PHE	CE1-CZ	5.18	1.47	1.37
1	A	106	VAL	C-O	5.17	1.33	1.23
1	A	49	ALA	N-CA	5.13	1.56	1.46
1	A	173	PRO	N-CD	5.12	1.55	1.47
1	A	232	ASN	CG-OD1	5.08	1.35	1.24
1	A	217	GLU	CD-OE2	5.06	1.31	1.25

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ARG	NE-CZ-NH1	25.18	132.89	120.30
1	A	116	ARG	NE-CZ-NH1	22.94	131.77	120.30
1	A	79	ARG	NE-CZ-NH1	22.87	131.73	120.30
1	A	150	ARG	NE-CZ-NH2	-21.54	109.53	120.30
1	A	249	TYR	CB-CG-CD1	-18.27	110.04	121.00
1	A	292	ASP	CB-CG-OD2	-15.67	104.20	118.30
1	A	67	ASP	CB-CG-OD1	14.65	131.48	118.30
1	A	291	ARG	NE-CZ-NH2	-13.85	113.38	120.30
1	A	235	ASP	CB-CG-OD1	13.67	130.60	118.30
1	A	120	GLU	OE1-CD-OE2	12.61	138.44	123.30
1	A	67	ASP	CB-CG-OD2	-11.81	107.67	118.30
1	A	149	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	A	150	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	A	128	ARG	NE-CZ-NH1	10.75	125.68	120.30
1	A	249	TYR	CG-CD1-CE1	-10.61	112.81	121.30
1	A	79	ARG	CG-CD-NE	10.21	133.24	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ASP	CB-CG-OD2	10.20	127.48	118.30
1	A	170	TYR	CB-CG-CD1	-10.09	114.95	121.00
1	A	221	PHE	CB-CG-CD1	-9.71	114.00	120.80
1	A	296	GLU	OE1-CD-OE2	9.37	134.55	123.30
1	A	235	ASP	CB-CG-OD2	-9.17	110.05	118.30
1	A	201	ILE	CB-CG1-CD1	9.11	139.42	113.90
1	A	149	ARG	NH1-CZ-NH2	8.96	129.26	119.40
1	A	116	ARG	NH1-CZ-NH2	-8.91	109.60	119.40
1	A	79	ARG	NH1-CZ-NH2	-8.85	109.67	119.40
1	A	249	TYR	CD1-CG-CD2	8.68	127.45	117.90
1	A	300	LYS	CA-CB-CG	8.57	132.25	113.40
1	A	149	ARG	NE-CZ-NH1	-8.55	116.03	120.30
1	A	101	ASP	CB-CG-OD1	8.53	125.97	118.30
1	A	268	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	A	257	ASP	CB-CG-OD2	7.99	125.49	118.30
1	A	256	PRO	O-C-N	-7.96	109.96	122.70
1	A	248	PHE	CB-CG-CD2	-7.93	115.25	120.80
1	A	178	ASP	CB-CG-OD2	7.91	125.42	118.30
1	A	34	GLU	OE1-CD-OE2	7.90	132.78	123.30
1	A	221	PHE	CB-CG-CD2	7.88	126.32	120.80
1	A	77	LYS	CA-CB-CG	7.82	130.61	113.40
1	A	268	TYR	CG-CD2-CE2	-7.81	115.06	121.30
1	A	61	PHE	CB-CG-CD2	-7.70	115.41	120.80
1	A	300	LYS	N-CA-CB	7.68	124.42	110.60
1	A	151	ARG	NE-CZ-NH2	7.65	124.12	120.30
1	A	188	SER	O-C-N	-7.45	110.79	122.70
1	A	239	GLU	OE1-CD-OE2	-7.38	114.45	123.30
1	A	217	GLU	CG-CD-OE1	7.30	132.90	118.30
1	A	144	GLU	CG-CD-OE1	7.26	132.82	118.30
1	A	12	PRO	N-CD-CG	-7.22	92.37	103.20
1	A	141	THR	CA-CB-CG2	7.20	122.48	112.40
1	A	151	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	120	GLU	CG-CD-OE2	-7.17	103.97	118.30
1	A	294	PHE	CB-CG-CD1	-7.05	115.86	120.80
1	A	296	GLU	CB-CA-C	-7.01	96.39	110.40
1	A	150	ARG	CA-CB-CG	-6.92	98.17	113.40
1	A	79	ARG	CA-CB-CG	6.91	128.59	113.40
1	A	166	GLU	OE1-CD-OE2	6.91	131.59	123.30
1	A	296	GLU	CG-CD-OE2	-6.85	104.60	118.30
1	A	146	ASP	O-C-N	6.84	133.64	122.70
1	A	249	TYR	CZ-CE2-CD2	-6.82	113.67	119.80
1	A	103	VAL	CA-CB-CG1	6.81	121.11	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ILE	C-N-CA	6.78	138.64	121.70
1	A	151	ARG	NH1-CZ-NH2	-6.77	111.96	119.40
1	A	130	TRP	CB-CG-CD2	-6.74	117.84	126.60
1	A	124	GLU	OE1-CD-OE2	6.66	131.29	123.30
1	A	138	MET	CB-CG-SD	-6.65	92.45	112.40
1	A	61	PHE	CD1-CG-CD2	6.50	126.75	118.30
1	A	290	THR	CA-CB-CG2	6.45	121.43	112.40
1	A	242	LYS	CD-CE-NZ	-6.44	96.89	111.70
1	A	130	TRP	CB-CG-CD1	6.41	135.34	127.00
1	A	276	GLU	OE1-CD-OE2	6.33	130.89	123.30
1	A	64	CYS	N-CA-CB	6.30	121.93	110.60
1	A	184	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	110	ALA	O-C-N	-6.21	112.76	122.70
1	A	150	ARG	CD-NE-CZ	6.21	132.29	123.60
1	A	96	LYS	O-C-N	-6.13	112.78	123.20
1	A	282	GLU	CG-CD-OE1	-6.10	106.10	118.30
1	A	22	LYS	CG-CD-CE	-6.06	93.72	111.90
1	A	188	SER	CA-C-N	5.99	130.38	117.20
1	A	274	ASP	O-C-N	-5.98	113.13	122.70
1	A	302	GLY	O-C-N	-5.97	113.15	122.70
1	A	292	ASP	OD1-CG-OD2	5.96	134.61	123.30
1	A	297	GLU	CA-C-N	5.95	130.29	117.20
1	A	112	LYS	CD-CE-NZ	-5.88	98.17	111.70
1	A	111	THR	O-C-N	5.85	132.06	122.70
1	A	116	ARG	CG-CD-NE	-5.85	99.51	111.80
1	A	296	GLU	N-CA-CB	5.84	121.12	110.60
1	A	4	LYS	CA-CB-CG	-5.78	100.68	113.40
1	A	269	ASN	OD1-CG-ND2	5.76	135.16	121.90
1	A	141	THR	CA-CB-OG1	-5.75	96.93	109.00
1	A	42	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	157	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	236	ALA	O-C-N	5.67	131.78	122.70
1	A	7	PHE	CZ-CE2-CD2	5.67	126.91	120.10
1	A	88	VAL	C-N-CA	5.67	135.87	121.70
1	A	170	TYR	CB-CG-CD2	5.66	124.40	121.00
1	A	99	PRO	N-CD-CG	-5.64	94.73	103.20
1	A	170	TYR	CD1-CE1-CZ	-5.62	114.75	119.80
1	A	283	VAL	CA-CB-CG2	5.61	119.32	110.90
1	A	288	LEU	O-C-N	-5.58	113.78	122.70
1	A	269	ASN	CB-CG-OD1	-5.56	110.48	121.60
1	A	259	HIS	CA-C-N	5.55	127.30	116.20
1	A	117	GLN	CG-CD-OE1	-5.53	110.53	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ARG	O-C-N	5.52	131.54	122.70
1	A	199	TRP	CD1-NE1-CE2	-5.51	104.04	109.00
1	A	193	HIS	CA-CB-CG	-5.50	104.25	113.60
1	A	215	ALA	O-C-N	-5.46	113.96	122.70
1	A	37	LYS	CG-CD-CE	5.46	128.26	111.90
1	A	124	GLU	O-C-N	-5.44	114.00	122.70
1	A	137	VAL	CG1-CB-CG2	5.39	119.52	110.90
1	A	144	GLU	CG-CD-OE2	-5.38	107.53	118.30
1	A	241	SER	CA-CB-OG	-5.38	96.66	111.20
1	A	100	MET	O-C-N	-5.37	114.12	122.70
1	A	260	GLY	O-C-N	-5.33	114.18	122.70
1	A	213	VAL	O-C-N	5.31	131.20	122.70
1	A	7	PHE	CG-CD2-CE2	-5.31	114.96	120.80
1	A	248	PHE	CB-CG-CD1	5.30	124.51	120.80
1	A	214	ARG	CD-NE-CZ	-5.30	116.18	123.60
1	A	60	GLY	O-C-N	5.30	131.18	122.70
1	A	101	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	237	VAL	CA-C-O	-5.24	109.09	120.10
1	A	22	LYS	CB-CG-CD	-5.24	97.99	111.60
1	A	60	GLY	N-CA-C	-5.23	100.02	113.10
1	A	286	VAL	CA-CB-CG1	5.20	118.70	110.90
1	A	217	GLU	CG-CD-OE2	-5.20	107.90	118.30
1	A	127	LYS	CD-CE-NZ	-5.20	99.75	111.70
1	A	291	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	A	49	ALA	CA-C-O	-5.19	109.21	120.10
1	A	103	VAL	O-C-N	5.19	130.95	121.10
1	A	221	PHE	CD1-CE1-CZ	5.16	126.29	120.10
1	A	257	ASP	OD1-CG-OD2	-5.15	113.52	123.30
1	A	109	ALA	CA-C-N	5.13	128.50	117.20
1	A	131	ASP	CA-C-O	-5.12	109.35	120.10
1	A	143	ASN	OD1-CG-ND2	-5.11	110.15	121.90
1	A	274	ASP	CA-C-O	5.10	130.81	120.10
1	A	274	ASP	CA-CB-CG	-5.10	102.18	113.40
1	A	119	GLN	CG-CD-OE1	5.09	131.78	121.60
1	A	100	MET	C-N-CA	5.09	134.42	121.70
1	A	87	ALA	O-C-N	5.07	130.82	122.70
1	A	291	ARG	CB-CA-C	-5.07	100.25	110.40
1	A	281	THR	CA-C-N	5.06	128.33	117.20
1	A	210	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	A	30	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	A	249	TYR	O-C-N	-5.01	114.68	123.20

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	2320	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	2343	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: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: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:69:LYS:NZ	4:A:726:HOH:O	1.99	0.58
1:A:146:ASP:CG	4:A:741:HOH:O	2.38	0.56
1:A:257:ASP:OD2	1:A:301:LYS:NZ	2.35	0.56
1:A:99:PRO:HG3	4:A:739:HOH:O	2.06	0.56
1:A:270:TRP:NE1	1:A:276:GLU:OE1	2.41	0.54
1:A:296:GLU:CD	4:A:569:HOH:O	2.46	0.54
1:A:172:VAL:HB	1:A:189:MET:HE3	1.88	0.54
1:A:269:ASN:ND2	4:A:507:HOH:O	1.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:274:ASP:CG	4:A:764:HOH:O	2.44	0.50
1:A:171:GLN:HG3	4:A:450:HOH:O	2.12	0.50
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:112:LYS:HD3	1:A:112:LYS:HA	1.54	0.48
1:A:262:LYS:O	1:A:266:MET:HE2	2.14	0.48
1:A:295:LYS:CD	4:A:757:HOH:O	2.37	0.47
1:A:68:PRO:HB3	1:A:91:GLN:O	2.15	0.47
1:A:212:GLY:O	1:A:216:THR:HG23	2.15	0.46
1:A:273:LYS:O	1:A:274:ASP:C	2.54	0.45
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:122:TYR:CE1	1:A:125:MET:HE1	2.54	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:100:MET:HE3	1:A:100:MET:HB3	1.96	0.41
1:A:179:ILE:N	1:A:180:PRO:CD	2.83	0.41
1:A:167:LYS:O	1:A:167:LYS:HG3	2.19	0.41
1:A:16:TRP:CZ2	3:A:308[B]:FCB:H63	2.56	0.41
1:A:98:LYS:HA	1:A:99:PRO:HD3	1.82	0.41
1:A:134:GLU:HG2	1:A:134:GLU:H	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 ⓘ

### 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%)	295 (97%)	5 (2%)	3 (1%)	19 7

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 ⓘ

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%)	230 (95%)	13 (5%)	28 16

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	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

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

### 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 carbohydrates 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	$\# Z  > 2$
2	FCA	A	307[A]	-	11,11,11	1.69	2 (18%)	16,16,16	1.01	0
3	FCB	A	308[B]	-	11,11,11	2.53	2 (18%)	16,16,16	1.37	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]	-	-	0/0/20/20	0/1/1/1
3	FCB	A	308[B]	-	-	0/0/20/20	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]	FCB	C3-C2	-6.03	1.36	1.52
2	A	307[A]	FCA	O2-C2	3.32	1.50	1.43
2	A	307[A]	FCA	O5-C1	3.71	1.50	1.43
3	A	308[B]	FCB	O3-C3	4.81	1.54	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	308[B]	FCB	C3-C4-C5	-2.75	105.08	109.72
3	A	308[B]	FCB	O3-C3-C4	-2.21	105.37	110.34
3	A	308[B]	FCB	C1-O5-C5	2.14	117.58	113.57

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 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.