



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:19 AM UTC

PDB ID : 6T2N / pdb_00006t2n
Title : Prominent members of the human gut microbiota express endo-acting O-glycanases to initiate mucin breakdown
Authors : Crouch, L.I.; Liberato, M.V.; Ubranowicz, P.A.; Basle, A.; Lamb, C.A.; Cooke, K.; Doona, M.; Needham, S.; Brady, R.R.; Berrington, J.E.; Madubic, K.; Chater, P.; Zhang, F.; Linhardt, R.J.; Spence, D.I.R.; Bolam, D.N.
Deposited on : 2019-10-09
Resolution : 2.70 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

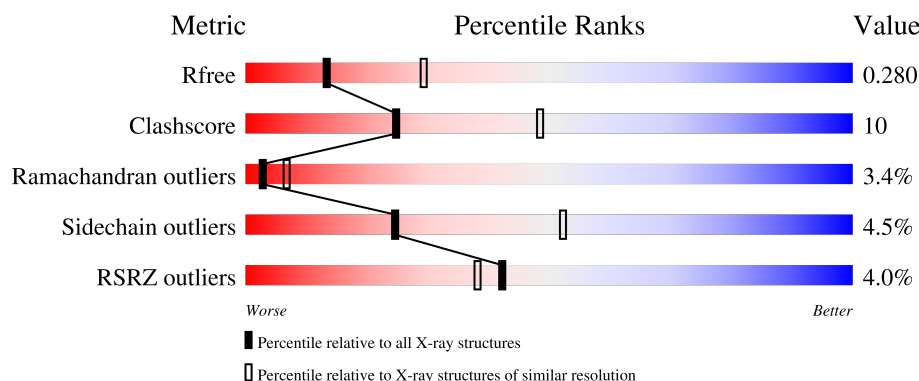
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	AAA	324	
1	BBB	324	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4472 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 Glycoside hydrolase family 16 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	278	Total	C	N	O	S	0	0	0
			2235	1434	381	412	8			
1	BBB	278	Total	C	N	O	S	0	0	0
			2235	1434	381	412	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-33	MET	-	initiating methionine	UNP A0A2N8IRP0
AAA	-32	GLY	-	expression tag	UNP A0A2N8IRP0
AAA	-31	SER	-	expression tag	UNP A0A2N8IRP0
AAA	-30	SER	-	expression tag	UNP A0A2N8IRP0
AAA	-29	HIS	-	expression tag	UNP A0A2N8IRP0
AAA	-28	HIS	-	expression tag	UNP A0A2N8IRP0
AAA	-27	HIS	-	expression tag	UNP A0A2N8IRP0
AAA	-26	HIS	-	expression tag	UNP A0A2N8IRP0
AAA	-25	HIS	-	expression tag	UNP A0A2N8IRP0
AAA	-24	HIS	-	expression tag	UNP A0A2N8IRP0
AAA	-23	SER	-	expression tag	UNP A0A2N8IRP0
AAA	-22	SER	-	expression tag	UNP A0A2N8IRP0
AAA	-21	GLY	-	expression tag	UNP A0A2N8IRP0
AAA	-20	LEU	-	expression tag	UNP A0A2N8IRP0
AAA	-19	VAL	-	expression tag	UNP A0A2N8IRP0
AAA	-18	PRO	-	expression tag	UNP A0A2N8IRP0
AAA	-17	ARG	-	expression tag	UNP A0A2N8IRP0
AAA	-16	GLY	-	expression tag	UNP A0A2N8IRP0
AAA	-15	SER	-	expression tag	UNP A0A2N8IRP0
AAA	-14	HIS	-	expression tag	UNP A0A2N8IRP0
AAA	172	THR	LYS	conflict	UNP A0A2N8IRP0
BBB	-33	MET	-	initiating methionine	UNP A0A2N8IRP0
BBB	-32	GLY	-	expression tag	UNP A0A2N8IRP0
BBB	-31	SER	-	expression tag	UNP A0A2N8IRP0
BBB	-30	SER	-	expression tag	UNP A0A2N8IRP0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-29	HIS	-	expression tag	UNP A0A2N8IRP0
BBB	-28	HIS	-	expression tag	UNP A0A2N8IRP0
BBB	-27	HIS	-	expression tag	UNP A0A2N8IRP0
BBB	-26	HIS	-	expression tag	UNP A0A2N8IRP0
BBB	-25	HIS	-	expression tag	UNP A0A2N8IRP0
BBB	-24	HIS	-	expression tag	UNP A0A2N8IRP0
BBB	-23	SER	-	expression tag	UNP A0A2N8IRP0
BBB	-22	SER	-	expression tag	UNP A0A2N8IRP0
BBB	-21	GLY	-	expression tag	UNP A0A2N8IRP0
BBB	-20	LEU	-	expression tag	UNP A0A2N8IRP0
BBB	-19	VAL	-	expression tag	UNP A0A2N8IRP0
BBB	-18	PRO	-	expression tag	UNP A0A2N8IRP0
BBB	-17	ARG	-	expression tag	UNP A0A2N8IRP0
BBB	-16	GLY	-	expression tag	UNP A0A2N8IRP0
BBB	-15	SER	-	expression tag	UNP A0A2N8IRP0
BBB	-14	HIS	-	expression tag	UNP A0A2N8IRP0
BBB	172	THR	LYS	conflict	UNP A0A2N8IRP0

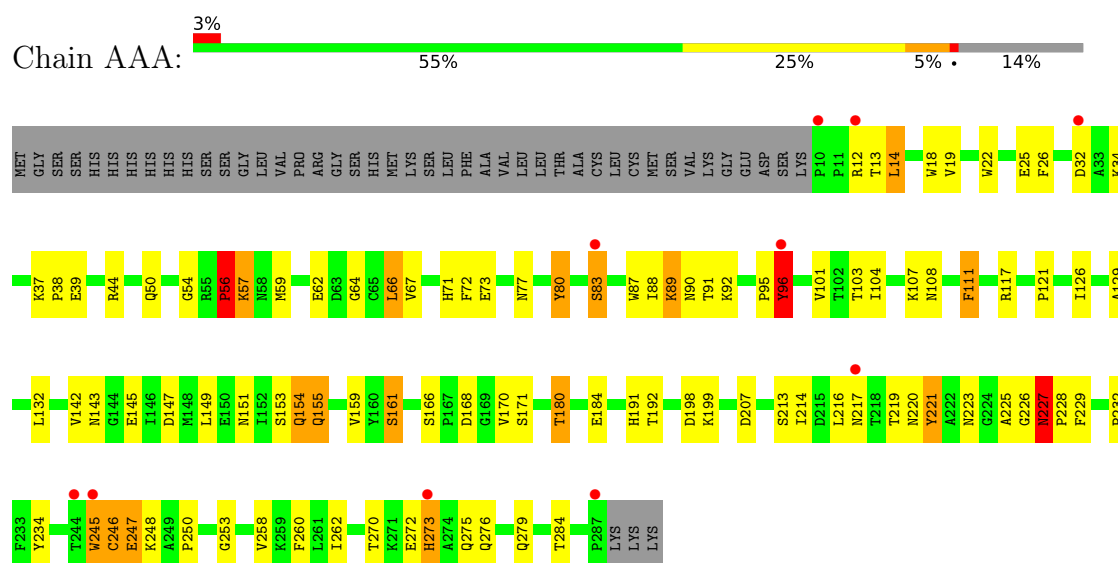
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Ca 1 1	0	0
2	BBB	1	Total Ca 1 1	0	0

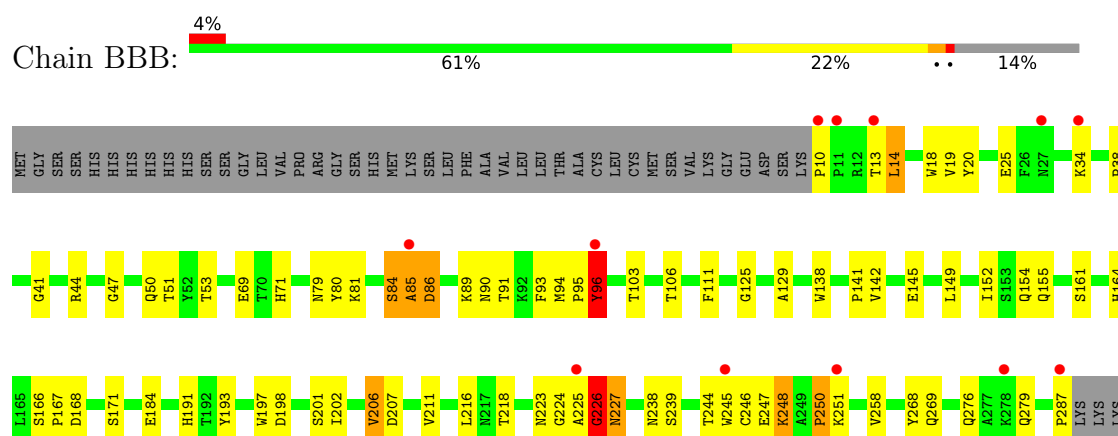
3 Residue-property plots [i](#)

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 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.

- Molecule 1: Glycoside hydrolase family 16 protein



- Molecule 1: Glycoside hydrolase family 16 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.47Å 96.13Å 128.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.72 – 2.70 19.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.72-2.70) 99.6 (19.72-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.233 , 0.281 0.237 , 0.280	Depositor DCC
R_{free} test set	1464 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	AAA	1.42	19/2299 (0.8%)	1.71	41/3117 (1.3%)
1	BBB	1.16	2/2299 (0.1%)	1.53	12/3117 (0.4%)
All	All	1.30	21/4598 (0.5%)	1.62	53/6234 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	2
1	BBB	0	3
All	All	0	5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	220	ASN	C-O	12.42	1.39	1.23
1	AAA	273	HIS	CG-CD2	8.88	1.45	1.35
1	AAA	273	HIS	ND1-CE1	8.48	1.41	1.32
1	AAA	56	PRO	C-N	-8.17	1.23	1.33
1	AAA	273	HIS	C-O	7.81	1.33	1.24
1	AAA	273	HIS	CB-CG	7.42	1.60	1.50
1	AAA	273	HIS	CD2-NE2	7.08	1.45	1.37
1	AAA	220	ASN	CG-ND2	-6.81	1.19	1.33
1	AAA	96	TYR	N-CA	6.68	1.54	1.46
1	AAA	32	ASP	CB-CG	6.67	1.68	1.52
1	AAA	217	ASN	CB-CG	6.43	1.68	1.52
1	AAA	217	ASN	C-O	-6.18	1.16	1.24
1	AAA	273	HIS	CE1-NE2	6.10	1.38	1.32
1	AAA	223	ASN	CA-C	5.89	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	111	PHE	C-O	5.54	1.30	1.24
1	AAA	250	PRO	C-O	-5.37	1.17	1.23
1	BBB	38	PRO	C-O	-5.26	1.17	1.23
1	AAA	57	LYS	N-CA	5.20	1.52	1.46
1	AAA	56	PRO	CA-C	5.16	1.61	1.52
1	AAA	66	LEU	C-O	5.05	1.29	1.23
1	BBB	53	THR	C-O	5.00	1.30	1.23

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	32	ASP	CA-CB-CG	9.63	122.23	112.60
1	AAA	217	ASN	CA-CB-CG	-8.86	103.74	112.60
1	AAA	217	ASN	OD1-CG-ND2	-8.74	113.86	122.60
1	AAA	57	LYS	O-C-N	8.36	130.98	122.12
1	AAA	56	PRO	O-C-N	-8.27	111.15	122.24
1	AAA	44	ARG	CG-CD-NE	-7.98	94.44	112.00
1	BBB	250	PRO	N-CA-C	7.88	124.28	113.65
1	AAA	54	GLY	CA-C-N	7.61	130.96	120.39
1	AAA	54	GLY	C-N-CA	7.61	130.96	120.39
1	AAA	13	THR	CA-CB-OG1	-7.33	98.61	109.60
1	AAA	248	LYS	CB-CA-C	7.32	121.61	109.53
1	BBB	227	ASN	CA-CB-CG	-7.08	105.52	112.60
1	AAA	198	ASP	CB-CA-C	-7.04	96.30	111.78
1	AAA	223	ASN	CA-C-O	6.74	130.15	120.51
1	AAA	80	TYR	CA-C-O	-6.68	113.42	120.63
1	AAA	56	PRO	CA-C-N	6.52	129.31	120.38
1	AAA	56	PRO	C-N-CA	6.52	129.31	120.38
1	AAA	199	LYS	CB-CA-C	-6.38	97.98	110.11
1	AAA	95	PRO	N-CA-C	-6.36	99.36	112.47
1	BBB	250	PRO	CA-C-N	-6.22	117.09	126.86
1	BBB	250	PRO	C-N-CA	-6.22	117.09	126.86
1	AAA	57	LYS	N-CA-C	-6.22	103.80	111.33
1	AAA	273	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
1	AAA	220	ASN	CB-CG-ND2	6.17	125.66	116.40
1	AAA	151	ASN	CA-C-O	-6.08	113.67	120.66
1	AAA	260	PHE	CA-CB-CG	6.03	119.83	113.80
1	AAA	25	GLU	N-CA-C	-5.99	106.01	113.38
1	AAA	44	ARG	CB-CA-C	-5.84	97.18	109.38
1	AAA	199	LYS	O-C-N	5.80	130.97	122.39
1	AAA	32	ASP	CB-CA-C	5.74	120.27	110.81
1	AAA	56	PRO	N-CA-C	-5.66	106.48	113.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	220	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	AAA	221	TYR	CA-C-O	-5.62	114.65	121.28
1	AAA	273	HIS	CG-CD2-NE2	5.59	112.79	107.20
1	AAA	96	TYR	CB-CA-C	-5.59	99.30	110.42
1	BBB	152	ILE	CA-C-N	5.59	130.08	121.19
1	BBB	152	ILE	C-N-CA	5.59	130.08	121.19
1	BBB	86	ASP	CA-CB-CG	5.56	118.16	112.60
1	BBB	93	PHE	CA-C-O	-5.48	114.91	121.11
1	AAA	88	ILE	CA-C-N	5.39	128.25	120.38
1	AAA	88	ILE	C-N-CA	5.39	128.25	120.38
1	AAA	34	LYS	N-CA-C	-5.29	106.83	113.28
1	AAA	154	GLN	CB-CA-C	5.17	119.35	110.81
1	BBB	91	THR	CA-CB-OG1	-5.13	101.91	109.60
1	AAA	39	GLU	CA-C-O	-5.08	115.63	121.47
1	AAA	245	TRP	CA-C-N	5.07	131.23	121.54
1	AAA	245	TRP	C-N-CA	5.07	131.23	121.54
1	BBB	79	ASN	CA-C-N	5.06	131.20	121.54
1	BBB	79	ASN	C-N-CA	5.06	131.20	121.54
1	BBB	184	GLU	CB-CA-C	5.05	117.78	109.90
1	AAA	25	GLU	CB-CA-C	5.03	118.41	109.65
1	AAA	221	TYR	CA-C-N	5.01	128.31	120.75
1	AAA	221	TYR	C-N-CA	5.01	128.31	120.75

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	143	ASN	Mainchain
1	AAA	56	PRO	Mainchain
1	BBB	226	GLY	Peptide
1	BBB	84	SER	Peptide
1	BBB	96	TYR	Sidechain

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	AAA	2235	0	2193	45	0
1	BBB	2235	0	2193	43	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
All	All	4472	0	4386	87	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 10.

All (87) 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:BBB:80:TYR:O	1:BBB:89:LYS:O	1.82	0.96
1:AAA:226:GLY:O	1:AAA:284:THR:O	1.84	0.93
1:BBB:250:PRO:O	1:BBB:251:LYS:HB2	1.78	0.82
1:BBB:71:HIS:O	1:BBB:96:TYR:HA	1.86	0.76
1:AAA:80:TYR:O	1:AAA:89:LYS:O	2.07	0.72
1:AAA:56:PRO:HA	1:AAA:59:MET:O	1.89	0.72
1:AAA:166:SER:OG	1:AAA:168:ASP:O	2.11	0.68
1:BBB:191:HIS:HD2	1:BBB:207:ASP:OD2	1.76	0.67
1:AAA:62:GLU:HB2	1:AAA:67:VAL:HG21	1.81	0.62
1:AAA:90:ASN:OD1	1:BBB:171:SER:HA	2.00	0.62
1:AAA:276:GLN:O	1:AAA:279:GLN:HG2	2.00	0.61
1:BBB:85:ALA:O	1:BBB:86:ASP:HB3	2.02	0.60
1:AAA:121:PRO:CB	1:AAA:258:VAL:HG13	2.33	0.59
1:BBB:161:SER:HB2	1:BBB:211:VAL:CG1	2.34	0.58
1:AAA:50:GLN:HA	1:AAA:96:TYR:O	2.05	0.57
1:BBB:224:GLY:O	1:BBB:226:GLY:N	2.38	0.56
1:BBB:84:SER:C	1:BBB:85:ALA:O	2.47	0.56
1:BBB:216:LEU:C	1:BBB:218:THR:H	2.12	0.55
1:AAA:80:TYR:CD1	1:AAA:92:LYS:HA	2.41	0.55
1:BBB:41:GLY:HA2	1:BBB:51:THR:OG1	2.06	0.55
1:AAA:72:PHE:CG	1:AAA:253:GLY:HA3	2.42	0.54
1:BBB:129:ALA:HB3	1:BBB:238:ASN:OD1	2.07	0.54
1:BBB:84:SER:O	1:BBB:90:ASN:HB3	2.08	0.54
1:BBB:166:SER:HB2	1:BBB:171:SER:O	2.09	0.53
1:AAA:121:PRO:HB2	1:AAA:258:VAL:HG13	1.90	0.53
1:BBB:154:GLN:O	1:BBB:155:GLN:HB2	2.09	0.53
1:AAA:87:TRP:O	1:AAA:91:THR:OG1	2.23	0.53
1:AAA:38:PRO:HB3	1:AAA:59:MET:HE1	1.91	0.52
1:AAA:246:CYS:O	1:AAA:247:GLU:C	2.53	0.51
1:AAA:270:THR:OG1	1:AAA:272:GLU:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:18:TRP:CH2	1:AAA:273:HIS:CE1	2.98	0.51
1:BBB:19:VAL:HG12	1:BBB:269:GLN:O	2.11	0.50
1:BBB:14:LEU:HB2	1:BBB:18:TRP:HB2	1.93	0.50
1:BBB:166:SER:CB	1:BBB:171:SER:O	2.60	0.50
1:AAA:132:LEU:HA	1:AAA:234:TYR:O	2.11	0.49
1:AAA:108:ASN:HB3	1:AAA:232:PRO:HB2	1.93	0.49
1:BBB:13:THR:HG22	1:BBB:14:LEU:O	2.13	0.49
1:AAA:22:TRP:CD1	1:AAA:107:LYS:HD3	2.47	0.49
1:BBB:161:SER:HB2	1:BBB:211:VAL:HG11	1.95	0.48
1:BBB:103:THR:HA	1:BBB:106:THR:OG1	2.13	0.48
1:AAA:57:LYS:HZ3	1:AAA:73:GLU:CD	2.21	0.48
1:AAA:214:ILE:HD11	1:AAA:219:THR:HG21	1.94	0.48
1:AAA:121:PRO:HB3	1:AAA:258:VAL:HG13	1.95	0.48
1:AAA:142:VAL:HG22	1:AAA:166:SER:HB3	1.96	0.48
1:AAA:14:LEU:HB2	1:AAA:18:TRP:HB2	1.94	0.48
1:AAA:103:THR:O	1:AAA:104:ILE:C	2.57	0.48
1:AAA:57:LYS:HG2	1:AAA:71:HIS:CD2	2.50	0.47
1:BBB:198:ASP:HB3	1:BBB:201:SER:H	1.80	0.47
1:BBB:276:GLN:O	1:BBB:279:GLN:HG2	2.15	0.47
1:BBB:145:GLU:HB3	1:BBB:164:HIS:HB2	1.97	0.47
1:AAA:145:GLU:OE2	1:AAA:147:ASP:OD1	2.32	0.46
1:BBB:149:LEU:HD22	1:BBB:193:TYR:CZ	2.51	0.46
1:AAA:170:VAL:HG12	1:AAA:171:SER:N	2.29	0.46
1:AAA:166:SER:HB2	1:AAA:171:SER:O	2.16	0.46
1:BBB:125:GLY:HA2	1:BBB:247:GLU:O	2.15	0.46
1:AAA:221:TYR:CE2	1:AAA:228:PRO:HD3	2.50	0.46
1:AAA:117:ARG:HD2	1:AAA:192:THR:OG1	2.15	0.45
1:BBB:50:GLN:HA	1:BBB:96:TYR:O	2.16	0.45
1:AAA:147:ASP:O	1:AAA:161:SER:HA	2.17	0.45
1:BBB:69:GLU:HG2	1:BBB:71:HIS:NE2	2.31	0.45
1:BBB:129:ALA:HA	1:BBB:149:LEU:O	2.17	0.45
1:BBB:47:GLY:O	1:BBB:248:LYS:HE3	2.17	0.44
1:BBB:10:PRO:HB3	1:BBB:25:GLU:OE2	2.17	0.44
1:AAA:191:HIS:HD2	1:AAA:207:ASP:OD2	2.01	0.44
1:AAA:66:LEU:HD23	1:AAA:262:ILE:HD13	1.99	0.43
1:AAA:154:GLN:O	1:AAA:155:GLN:HB2	2.18	0.43
1:BBB:84:SER:OG	1:BBB:89:LYS:HB2	2.18	0.43
1:AAA:57:LYS:NZ	1:AAA:73:GLU:CD	2.76	0.43
1:AAA:126:ILE:HD12	1:AAA:126:ILE:HA	1.82	0.42
1:BBB:197:TRP:CD1	1:BBB:202:ILE:HG12	2.53	0.42
1:AAA:77:ASN:O	1:AAA:80:TYR:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:37:LYS:O	1:AAA:101:VAL:HA	2.19	0.42
1:BBB:138:TRP:HB3	1:BBB:142:VAL:HB	2.01	0.42
1:BBB:95:PRO:O	1:BBB:96:TYR:O	2.37	0.41
1:AAA:153:SER:HB2	1:AAA:247:GLU:OE1	2.20	0.41
1:BBB:20:TYR:HB2	1:BBB:268:TYR:CE1	2.55	0.41
1:AAA:227:ASN:HD22	1:AAA:229:PHE:H	1.67	0.41
1:BBB:193:TYR:CE2	1:BBB:206:VAL:HG13	2.56	0.41
1:BBB:245:TRP:O	1:BBB:246:CYS:C	2.64	0.41
1:BBB:69:GLU:HG2	1:BBB:71:HIS:CD2	2.55	0.41
1:BBB:10:PRO:HG3	1:BBB:25:GLU:HG3	2.02	0.41
1:AAA:129:ALA:HA	1:AAA:149:LEU:O	2.21	0.40
1:BBB:245:TRP:CE3	1:BBB:245:TRP:HA	2.56	0.40
1:BBB:216:LEU:C	1:BBB:218:THR:N	2.79	0.40
1:AAA:26:PHE:O	1:AAA:64:GLY:HA2	2.21	0.40
1:AAA:159:VAL:O	1:AAA:180:THR:HA	2.21	0.40
1:BBB:94:MET:C	1:BBB:95:PRO:O	2.60	0.40

There are no symmetry-related clashes.

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	AAA	276/324 (85%)	243 (88%)	24 (9%)	9 (3%)	3	7
1	BBB	276/324 (85%)	240 (87%)	26 (9%)	10 (4%)	2	6
All	All	552/648 (85%)	483 (88%)	50 (9%)	19 (3%)	3	7

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	83	SER
1	AAA	225	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AAA	246	CYS
1	AAA	247	GLU
1	BBB	81	LYS
1	BBB	96	TYR
1	BBB	225	ALA
1	AAA	96	TYR
1	BBB	85	ALA
1	BBB	111	PHE
1	BBB	223	ASN
1	AAA	14	LEU
1	AAA	227	ASN
1	BBB	167	PRO
1	BBB	226	GLY
1	AAA	111	PHE
1	AAA	155	GLN
1	BBB	14	LEU
1	BBB	227	ASN

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	AAA	242/282 (86%)	230 (95%)	12 (5%)	22	48
1	BBB	242/282 (86%)	232 (96%)	10 (4%)	27	56
All	All	484/564 (86%)	462 (96%)	22 (4%)	24	52

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	12	ARG
1	AAA	19	VAL
1	AAA	83	SER
1	AAA	89	LYS
1	AAA	161	SER
1	AAA	180	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AAA	184	GLU
1	AAA	213	SER
1	AAA	216	LEU
1	AAA	227	ASN
1	AAA	245	TRP
1	AAA	275	GLN
1	BBB	34	LYS
1	BBB	44	ARG
1	BBB	141	PRO
1	BBB	168	ASP
1	BBB	206	VAL
1	BBB	239	SER
1	BBB	244	THR
1	BBB	248	LYS
1	BBB	258	VAL
1	BBB	287	PRO

Sometimes 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 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	278/324 (85%)	0.37	10 (3%) 46 42	47, 70, 98, 127	0
1	BBB	278/324 (85%)	0.42	12 (4%) 40 36	52, 75, 100, 119	0
All	All	556/648 (85%)	0.39	22 (3%) 42 38	47, 73, 100, 127	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	13	THR	4.6
1	AAA	10	PRO	4.5
1	BBB	85	ALA	3.9
1	BBB	10	PRO	3.8
1	BBB	287	PRO	3.7
1	AAA	273	HIS	3.0
1	AAA	12	ARG	2.8
1	AAA	217	ASN	2.7
1	AAA	96	TYR	2.7
1	BBB	225	ALA	2.7
1	AAA	245	TRP	2.6
1	BBB	251	LYS	2.4
1	BBB	278	LYS	2.4
1	BBB	34	LYS	2.3
1	AAA	244	THR	2.2
1	BBB	96	TYR	2.2
1	AAA	287	PRO	2.2
1	BBB	11	PRO	2.2
1	AAA	83	SER	2.2
1	BBB	27	ASN	2.1
1	BBB	245	TRP	2.1
1	AAA	32	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	BBB	401	1/1	0.91	0.14	106,106,106,106	0
2	CA	AAA	401	1/1	0.92	0.09	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.