



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 2QVC / pdb_00002qvc
Title : Crystal structure of a periplasmic sugar ABC transporter from *Thermotoga maritima*
Authors : Palani, K.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-08-08
Resolution : 2.40 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)	:	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

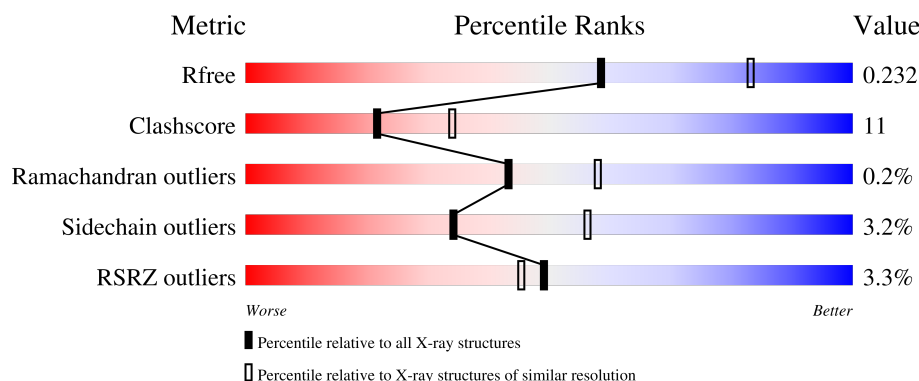
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	A	313	% 75% 20% • •
1	B	313	6% 70% 24% • •
1	C	313	4% 73% 20% • •
1	D	313	% 75% 19% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9455 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 Sugar ABC transporter, periplasmic sugar-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	Se	0	0	0
			2280	1461	366	441	1	11			
1	B	302	Total	C	N	O	S	Se	0	0	0
			2280	1461	366	441	1	11			
1	C	302	Total	C	N	O	S	Se	0	0	0
			2280	1461	366	441	1	11			
1	D	302	Total	C	N	O	S	Se	0	0	0
			2280	1461	366	441	1	11			

There are 44 discrepancies between the modelled and reference sequences:

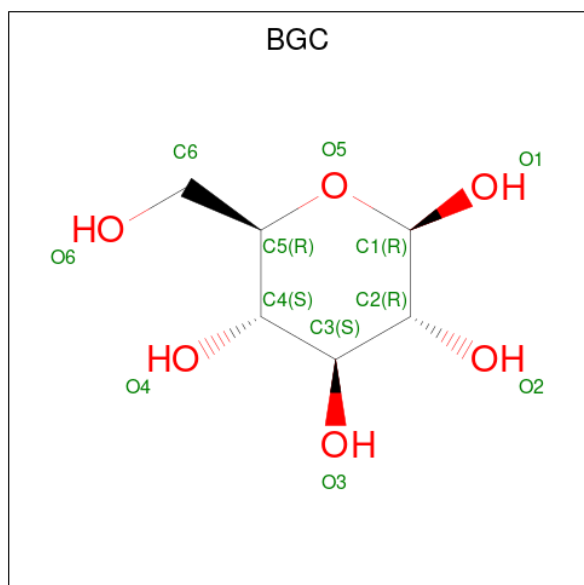
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MSE	-	expression tag	UNP Q9WXW9
A	31	SER	-	expression tag	UNP Q9WXW9
A	32	LEU	-	expression tag	UNP Q9WXW9
A	335	GLU	-	expression tag	UNP Q9WXW9
A	336	GLY	-	expression tag	UNP Q9WXW9
A	337	HIS	-	expression tag	UNP Q9WXW9
A	338	HIS	-	expression tag	UNP Q9WXW9
A	339	HIS	-	expression tag	UNP Q9WXW9
A	340	HIS	-	expression tag	UNP Q9WXW9
A	341	HIS	-	expression tag	UNP Q9WXW9
A	342	HIS	-	expression tag	UNP Q9WXW9
B	30	MSE	-	expression tag	UNP Q9WXW9
B	31	SER	-	expression tag	UNP Q9WXW9
B	32	LEU	-	expression tag	UNP Q9WXW9
B	335	GLU	-	expression tag	UNP Q9WXW9
B	336	GLY	-	expression tag	UNP Q9WXW9
B	337	HIS	-	expression tag	UNP Q9WXW9
B	338	HIS	-	expression tag	UNP Q9WXW9
B	339	HIS	-	expression tag	UNP Q9WXW9
B	340	HIS	-	expression tag	UNP Q9WXW9
B	341	HIS	-	expression tag	UNP Q9WXW9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	342	HIS	-	expression tag	UNP Q9WXW9
C	30	MSE	-	expression tag	UNP Q9WXW9
C	31	SER	-	expression tag	UNP Q9WXW9
C	32	LEU	-	expression tag	UNP Q9WXW9
C	335	GLU	-	expression tag	UNP Q9WXW9
C	336	GLY	-	expression tag	UNP Q9WXW9
C	337	HIS	-	expression tag	UNP Q9WXW9
C	338	HIS	-	expression tag	UNP Q9WXW9
C	339	HIS	-	expression tag	UNP Q9WXW9
C	340	HIS	-	expression tag	UNP Q9WXW9
C	341	HIS	-	expression tag	UNP Q9WXW9
C	342	HIS	-	expression tag	UNP Q9WXW9
D	30	MSE	-	expression tag	UNP Q9WXW9
D	31	SER	-	expression tag	UNP Q9WXW9
D	32	LEU	-	expression tag	UNP Q9WXW9
D	335	GLU	-	expression tag	UNP Q9WXW9
D	336	GLY	-	expression tag	UNP Q9WXW9
D	337	HIS	-	expression tag	UNP Q9WXW9
D	338	HIS	-	expression tag	UNP Q9WXW9
D	339	HIS	-	expression tag	UNP Q9WXW9
D	340	HIS	-	expression tag	UNP Q9WXW9
D	341	HIS	-	expression tag	UNP Q9WXW9
D	342	HIS	-	expression tag	UNP Q9WXW9

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



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

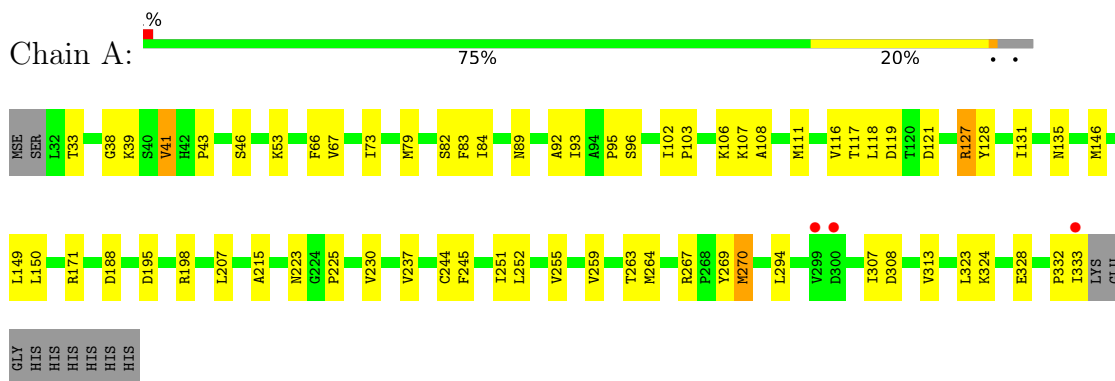
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total	O	0	0
			83	83		
3	B	63	Total	O	0	0
			63	63		
3	C	60	Total	O	0	0
			60	60		
3	D	81	Total	O	0	0
			81	81		

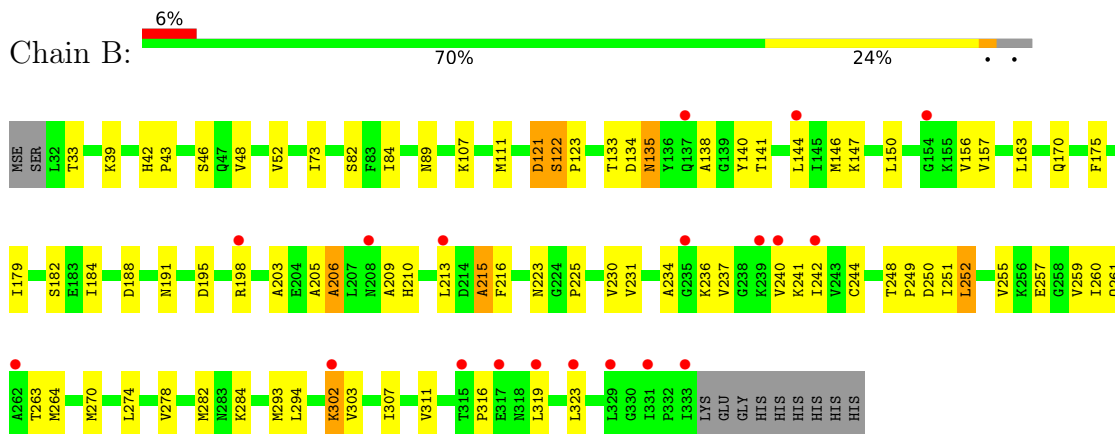
3 Residue-property plots [i](#)

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.

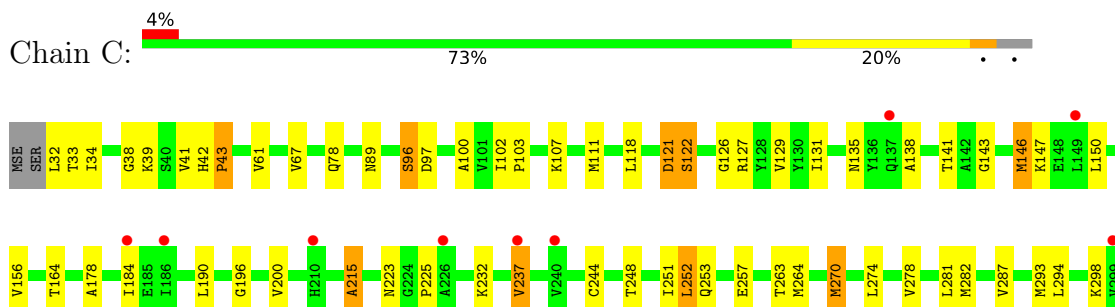
- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

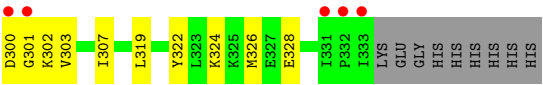


- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

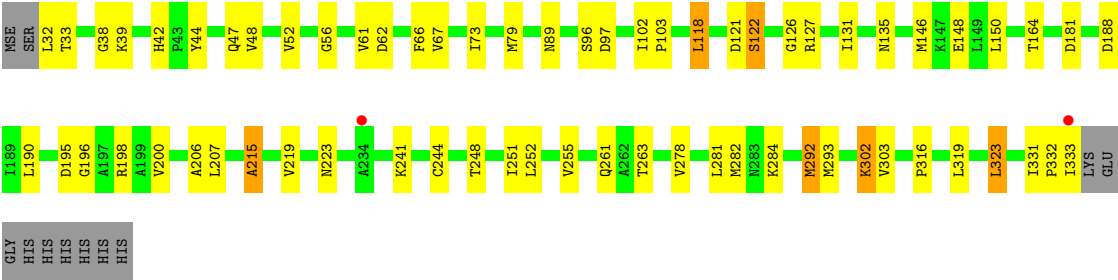
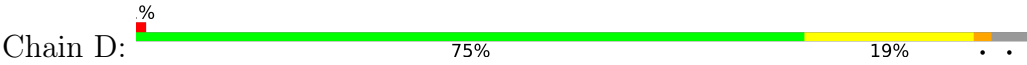


- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein





● Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	123.33Å 123.33Å 280.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.83 – 2.40 30.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.83-2.40) 93.1 (30.83-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.243 0.204 , 0.232	Depositor DCC
R_{free} test set	2924 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9455	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: BGC

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	0.51	0/2306	1.01	7/3110 (0.2%)
1	B	0.48	0/2306	1.04	12/3110 (0.4%)
1	C	0.46	0/2306	0.98	8/3110 (0.3%)
1	D	0.48	0/2306	0.99	9/3110 (0.3%)
All	All	0.48	0/9224	1.00	36/12440 (0.3%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ASN	N-CA-C	8.58	120.25	111.07
1	B	209	ALA	N-CA-C	-8.47	102.11	114.39
1	B	121	ASP	N-CA-C	7.29	121.18	110.17
1	C	121	ASP	N-CA-C	6.85	120.52	110.17
1	B	206	ALA	N-CA-C	-6.72	106.03	114.56
1	C	223	ASN	N-CA-C	6.68	118.25	110.97
1	C	122	SER	CA-C-N	6.62	127.15	119.47
1	C	122	SER	C-N-CA	6.62	127.15	119.47
1	B	223	ASN	N-CA-C	6.55	118.08	111.07
1	D	122	SER	CA-C-N	6.45	126.95	119.47
1	D	122	SER	C-N-CA	6.45	126.95	119.47
1	B	122	SER	CA-C-N	6.43	127.88	119.84
1	B	122	SER	C-N-CA	6.43	127.88	119.84
1	B	284	LYS	N-CA-C	6.39	118.05	111.14
1	A	121	ASP	N-CA-C	6.30	120.19	110.42
1	D	284	LYS	N-CA-C	6.20	117.83	111.14
1	D	223	ASN	N-CA-C	6.13	117.65	110.97
1	A	215	ALA	N-CA-C	6.10	118.12	108.79
1	D	135	ASN	N-CA-C	6.07	118.68	111.33
1	A	135	ASN	N-CA-C	6.06	118.38	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ALA	N-CA-C	5.97	118.14	109.07
1	C	96	SER	N-CA-C	-5.89	105.35	112.54
1	C	126	GLY	N-CA-C	-5.84	106.97	114.85
1	A	96	SER	N-CA-C	-5.83	106.12	113.18
1	A	332	PRO	N-CA-C	5.75	120.25	111.34
1	C	215	ALA	N-CA-C	5.74	117.83	108.76
1	C	135	ASN	N-CA-C	5.66	117.90	111.11
1	B	135	ASN	N-CA-C	5.56	117.34	111.28
1	A	128	TYR	N-CA-C	5.51	117.29	111.28
1	D	316	PRO	N-CA-C	-5.39	106.50	113.57
1	B	205	ALA	N-CA-C	-5.37	106.60	112.72
1	D	215	ALA	N-CA-C	5.20	116.43	108.42
1	D	126	GLY	N-CA-C	-5.19	107.95	115.27
1	B	46	SER	N-CA-C	-5.13	105.77	111.36
1	D	219	VAL	N-CA-C	5.10	115.87	110.72
1	B	293	MSE	N-CA-C	-5.03	107.31	113.50

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	2280	0	2331	43	0
1	B	2280	0	2331	59	0
1	C	2280	0	2331	56	0
1	D	2280	0	2331	50	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	83	0	0	8	0
3	B	63	0	0	1	0
3	C	60	0	0	2	0
3	D	81	0	0	3	0
All	All	9455	0	9372	200	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 11.

All (200) 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:B:107:LYS:HG2	1:B:111:MSE:HE2	1.32	1.04
1:D:146:MSE:HE2	1:D:150:LEU:HG	1.37	1.03
1:B:302:LYS:HZ2	1:B:303:VAL:H	1.04	0.97
1:A:33:THR:H	1:A:89:ASN:HD22	1.12	0.97
1:D:33:THR:H	1:D:89:ASN:HD22	1.10	0.94
1:B:107:LYS:HG2	1:B:111:MSE:CE	1.99	0.91
1:D:302:LYS:HZ2	1:D:303:VAL:H	0.93	0.89
1:C:33:THR:H	1:C:89:ASN:HD22	1.19	0.89
1:B:33:THR:H	1:B:89:ASN:HD22	1.16	0.86
1:D:33:THR:H	1:D:89:ASN:ND2	1.74	0.85
1:A:79:MSE:HE1	3:A:436:HOH:O	1.81	0.81
1:B:33:THR:H	1:B:89:ASN:ND2	1.81	0.78
1:B:302:LYS:HZ2	1:B:303:VAL:N	1.83	0.77
1:B:107:LYS:CG	1:B:111:MSE:HE2	2.11	0.77
1:C:33:THR:H	1:C:89:ASN:ND2	1.85	0.74
1:C:225:PRO:HD3	1:C:251:ILE:HG12	1.69	0.74
1:B:302:LYS:NZ	1:B:303:VAL:H	1.86	0.73
1:D:302:LYS:NZ	1:D:303:VAL:H	1.80	0.73
1:D:302:LYS:HZ2	1:D:303:VAL:N	1.79	0.73
1:B:231:VAL:HG13	1:B:236:LYS:HB2	1.72	0.71
1:A:33:THR:H	1:A:89:ASN:ND2	1.84	0.71
1:B:141:THR:CG2	1:B:264:MSE:HE1	2.22	0.69
1:A:117:THR:HG23	1:A:127:ARG:HG3	1.75	0.68
1:B:244:CYS:HB2	3:B:431:HOH:O	1.93	0.68
1:A:264:MSE:HE1	1:A:313:VAL:HG13	1.75	0.67
1:D:331:ILE:HG21	3:D:455:HOH:O	1.93	0.67
1:A:146:MSE:HE2	1:A:150:LEU:HG	1.75	0.67
1:A:127:ARG:O	1:A:127:ARG:HD3	1.97	0.65
1:D:38:GLY:HA3	1:D:67:VAL:HG12	1.77	0.65
1:A:146:MSE:HE3	1:A:146:MSE:HA	1.79	0.65
1:D:195:ASP:HB3	1:D:198:ARG:HB3	1.79	0.64
1:A:225:PRO:HD3	1:A:251:ILE:HG12	1.80	0.64
1:C:141:THR:HB	1:C:264:MSE:CE	2.29	0.63
1:B:236:LYS:HB3	1:B:240:VAL:HG23	1.80	0.63
1:A:79:MSE:HE3	1:A:82:SER:HB3	1.80	0.63
1:D:33:THR:N	1:D:89:ASN:HD22	1.90	0.63
1:A:267:ARG:HB3	1:A:270:MSE:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:HB2	1:B:259:VAL:HG23	1.81	0.61
1:C:146:MSE:HE3	1:C:146:MSE:HA	1.83	0.60
1:C:146:MSE:HE2	1:C:150:LEU:HG	1.83	0.60
1:C:253:GLN:O	1:C:257:GLU:HG3	2.00	0.60
1:C:42:HIS:HE1	1:C:248:THR:HG21	1.66	0.60
1:A:107:LYS:O	1:A:111:MSE:HG2	2.01	0.60
1:A:244:CYS:HB2	3:A:401:HOH:O	2.01	0.60
1:C:96:SER:O	1:C:164:THR:HG23	2.03	0.59
1:C:298:LYS:HE3	1:C:301:GLY:O	2.03	0.58
1:C:107:LYS:O	1:C:111:MSE:HG2	2.03	0.58
1:D:190:LEU:HD11	1:D:206:ALA:HB2	1.85	0.57
1:A:263:THR:C	1:A:264:MSE:HE2	2.28	0.57
1:C:232:LYS:HA	1:C:237:VAL:HG13	1.85	0.57
1:C:147:LYS:HA	1:C:184:ILE:HD11	1.86	0.57
1:D:146:MSE:HE2	1:D:150:LEU:CG	2.25	0.56
1:A:79:MSE:HE2	1:A:83:PHE:CE1	2.41	0.56
1:C:141:THR:HB	1:C:264:MSE:HE1	1.86	0.56
1:C:244:CYS:O	1:C:263:THR:HA	2.05	0.56
1:B:157:VAL:HG13	1:B:216:PHE:CD1	2.41	0.56
1:B:48:VAL:O	1:B:52:VAL:HG23	2.06	0.56
1:D:278:VAL:O	1:D:282:MSE:HG3	2.06	0.56
1:B:138:ALA:O	1:B:264:MSE:HE2	2.06	0.55
1:D:331:ILE:HD12	1:D:331:ILE:N	2.21	0.55
1:A:308:ASP:HA	3:A:441:HOH:O	2.06	0.55
1:B:206:ALA:O	1:B:210:HIS:HB2	2.07	0.55
1:C:278:VAL:HG22	1:D:293:MSE:HE3	1.89	0.55
1:C:244:CYS:HB2	3:C:403:HOH:O	2.07	0.54
1:C:232:LYS:HA	1:C:237:VAL:CG1	2.37	0.54
1:A:294:LEU:HD22	1:A:307:ILE:HD11	1.89	0.54
1:C:34:ILE:HG12	1:C:61:VAL:HG11	1.90	0.54
1:C:141:THR:CG2	1:C:264:MSE:HE1	2.38	0.54
1:C:127:ARG:HG2	1:C:127:ARG:HH11	1.72	0.54
1:B:244:CYS:O	1:B:263:THR:HA	2.08	0.53
1:D:244:CYS:HB2	3:D:412:HOH:O	2.09	0.53
1:B:203:ALA:HB3	1:B:230:VAL:HG21	1.91	0.53
1:C:294:LEU:HD21	1:D:293:MSE:CE	2.38	0.53
1:C:324:LYS:O	1:C:328:GLU:HG3	2.08	0.53
1:A:146:MSE:CE	1:A:149:LEU:HB2	2.39	0.53
1:C:38:GLY:HA3	1:C:67:VAL:HG12	1.91	0.53
1:B:278:VAL:O	1:B:282:MSE:HG3	2.09	0.53
1:A:38:GLY:HA3	1:A:67:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:HD22	1:B:307:ILE:HD11	1.92	0.53
1:D:96:SER:O	1:D:164:THR:HG23	2.10	0.53
1:B:146:MSE:HE3	1:B:146:MSE:HA	1.92	0.52
1:B:195:ASP:HB3	1:B:198:ARG:HB2	1.91	0.52
1:C:190:LEU:HD22	1:C:190:LEU:N	2.23	0.52
1:D:319:LEU:O	1:D:323:LEU:HD22	2.09	0.52
1:A:324:LYS:HE3	1:A:328:GLU:OE2	2.09	0.52
1:D:48:VAL:O	1:D:52:VAL:HG23	2.10	0.52
1:B:141:THR:HG22	1:B:264:MSE:HE1	1.92	0.52
1:B:141:THR:HB	1:B:264:MSE:CE	2.40	0.51
1:A:207:LEU:HD22	1:A:230:VAL:HG12	1.93	0.51
1:B:319:LEU:O	1:B:323:LEU:HD13	2.11	0.50
1:C:138:ALA:O	1:C:264:MSE:HE2	2.10	0.50
1:C:147:LYS:HD2	1:C:178:ALA:O	2.12	0.50
1:C:102:ILE:HB	1:C:103:PRO:HD3	1.93	0.50
1:C:156:VAL:HG23	1:C:215:ALA:O	2.12	0.50
1:C:270:MSE:O	1:C:274:LEU:HG	2.12	0.49
1:B:146:MSE:HE1	1:B:241:LYS:HB3	1.93	0.49
1:B:234:ALA:O	1:B:236:LYS:HG2	2.12	0.49
1:C:293:MSE:HE2	1:D:293:MSE:HE2	1.94	0.49
1:D:302:LYS:HZ3	1:D:302:LYS:HA	1.78	0.49
1:B:147:LYS:HE3	1:B:182:SER:HB3	1.95	0.49
1:D:196:GLY:O	1:D:200:VAL:HG23	2.13	0.49
1:C:129:VAL:HG23	1:C:282:MSE:HE1	1.94	0.49
1:D:73:ILE:HD13	1:D:97:ASP:HB2	1.94	0.49
1:A:195:ASP:HB3	1:A:198:ARG:HB3	1.94	0.49
1:A:84:ILE:CG2	1:A:111:MSE:HE2	2.43	0.48
1:A:146:MSE:HE3	1:A:149:LEU:HB2	1.95	0.48
1:C:294:LEU:HD22	1:C:307:ILE:HD11	1.94	0.48
1:D:207:LEU:HD23	1:D:207:LEU:O	2.13	0.48
1:A:333:ILE:HG22	1:A:333:ILE:O	2.13	0.48
1:C:293:MSE:HE1	1:D:281:LEU:CD1	2.44	0.48
1:D:32:LEU:HA	1:D:89:ASN:ND2	2.29	0.48
1:B:122:SER:N	1:B:123:PRO:HD3	2.29	0.48
1:B:141:THR:HB	1:B:264:MSE:HE1	1.96	0.47
1:C:97:ASP:HB3	1:C:100:ALA:HB3	1.97	0.47
1:C:127:ARG:HG2	1:C:127:ARG:NH1	2.29	0.47
1:C:32:LEU:HA	1:C:89:ASN:ND2	2.29	0.47
1:C:121:ASP:CG	1:C:122:SER:H	2.22	0.47
1:D:118:LEU:HA	1:D:131:ILE:O	2.14	0.47
1:A:84:ILE:HG22	1:A:111:MSE:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:O	1:A:95:PRO:HD3	2.14	0.47
1:A:237:VAL:HG13	1:A:259:VAL:HA	1.97	0.47
1:C:302:LYS:NZ	1:C:303:VAL:H	2.13	0.47
1:C:281:LEU:HD11	1:D:281:LEU:HD11	1.97	0.46
1:C:118:LEU:HA	1:C:131:ILE:O	2.16	0.46
1:A:269:TYR:HB3	3:A:437:HOH:O	2.15	0.46
1:B:261:GLN:O	1:B:316:PRO:HD3	2.14	0.46
1:C:143:GLY:HA3	1:C:178:ALA:HB3	1.97	0.46
1:D:38:GLY:CA	1:D:67:VAL:HG12	2.44	0.46
1:D:146:MSE:HE1	1:D:241:LYS:HB3	1.98	0.46
1:D:292:MSE:HE3	1:D:292:MSE:HA	1.97	0.46
1:B:135:ASN:HB2	1:B:170:GLN:OE1	2.16	0.45
1:A:251:ILE:O	1:A:255:VAL:HG23	2.17	0.45
1:C:293:MSE:HE1	1:D:281:LEU:HD11	1.98	0.45
1:D:146:MSE:HE3	1:D:146:MSE:HA	1.98	0.45
1:A:171:ARG:HD3	1:A:245:PHE:CZ	2.52	0.45
1:A:270:MSE:HG2	3:A:437:HOH:O	2.16	0.45
1:C:42:HIS:ND1	1:C:43:PRO:HD2	2.32	0.45
1:C:196:GLY:O	1:C:200:VAL:HG23	2.15	0.45
1:B:175:PHE:O	1:B:179:ILE:HG12	2.17	0.45
1:B:252:LEU:HG	1:B:319:LEU:HD11	1.98	0.45
1:D:102:ILE:HB	1:D:103:PRO:HD3	1.98	0.44
1:C:42:HIS:CE1	1:C:248:THR:HG21	2.48	0.44
1:C:156:VAL:HA	1:C:215:ALA:O	2.16	0.44
1:D:121:ASP:CG	1:D:122:SER:H	2.25	0.44
1:D:56:GLY:HA2	1:D:61:VAL:HG12	1.98	0.44
1:A:73:ILE:HD13	3:A:451:HOH:O	2.17	0.44
1:C:293:MSE:HE2	1:D:293:MSE:CE	2.47	0.44
1:D:244:CYS:O	1:D:263:THR:HA	2.17	0.44
1:B:156:VAL:HG22	1:B:215:ALA:HB3	1.99	0.43
1:B:244:CYS:SG	1:B:260:ILE:HD13	2.58	0.43
1:C:294:LEU:HD21	1:D:293:MSE:HE2	1.99	0.43
1:D:44:TYR:HA	1:D:47:GLN:HE21	1.83	0.43
1:B:146:MSE:HE2	1:B:150:LEU:HG	2.00	0.43
1:C:282:MSE:HG2	1:C:287:VAL:HA	2.00	0.43
1:D:261:GLN:N	1:D:261:GLN:CD	2.76	0.43
1:D:251:ILE:O	1:D:255:VAL:HG23	2.18	0.43
1:B:147:LYS:HA	1:B:184:ILE:HD11	2.00	0.43
1:C:33:THR:N	1:C:89:ASN:HD22	1.99	0.43
1:C:141:THR:CB	1:C:264:MSE:HE1	2.48	0.43
1:A:118:LEU:HA	1:A:131:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LEU:HG	1:C:319:LEU:HD11	2.01	0.43
1:B:251:ILE:O	1:B:255:VAL:HG23	2.19	0.42
1:D:332:PRO:O	1:D:333:ILE:HG22	2.18	0.42
1:B:133:THR:HG23	1:B:311:VAL:HG13	2.00	0.42
1:A:41:VAL:O	1:A:41:VAL:HG13	2.20	0.42
1:B:157:VAL:CG1	1:B:213:LEU:HD21	2.50	0.42
1:D:215:ALA:HB2	1:D:241:LYS:HB2	2.01	0.42
1:B:84:ILE:HG21	1:B:111:MSE:CE	2.50	0.42
1:B:141:THR:CB	1:B:264:MSE:HE1	2.49	0.42
1:B:248:THR:HB	1:B:249:PRO:HD2	2.02	0.42
1:B:274:LEU:O	1:B:278:VAL:HG23	2.20	0.42
1:A:102:ILE:HB	1:A:103:PRO:HD3	2.01	0.42
1:D:66:PHE:CD2	1:D:79:MSE:HG2	2.54	0.42
1:A:43:PRO:O	1:A:46:SER:HB2	2.19	0.42
1:B:33:THR:N	1:B:89:ASN:HD22	1.98	0.42
1:B:140:TYR:CE2	1:B:144:LEU:HD11	2.55	0.42
1:D:331:ILE:HG22	3:D:451:HOH:O	2.19	0.42
1:B:270:MSE:HE3	1:B:274:LEU:HG	2.02	0.42
1:D:42:HIS:HE1	1:D:248:THR:HG21	1.84	0.42
1:A:84:ILE:HD11	1:A:108:ALA:HB2	2.02	0.42
1:A:102:ILE:O	1:A:106:LYS:HG2	2.19	0.42
1:B:42:HIS:ND1	1:B:43:PRO:HD2	2.34	0.42
1:B:163:LEU:HG	1:B:191:ASN:HD22	1.85	0.42
1:B:242:ILE:HG21	1:B:260:ILE:HG12	2.01	0.42
1:C:300:ASP:HA	3:C:432:HOH:O	2.19	0.41
1:A:53:LYS:HD2	3:A:467:HOH:O	2.20	0.41
1:D:302:LYS:NZ	1:D:302:LYS:HA	2.36	0.41
1:B:198:ARG:NH1	1:B:198:ARG:HG2	2.35	0.41
1:D:56:GLY:HA2	1:D:61:VAL:CG1	2.49	0.41
1:A:92:ALA:HA	1:A:116:VAL:O	2.20	0.41
1:A:66:PHE:HA	3:A:446:HOH:O	2.21	0.41
1:C:147:LYS:HA	1:C:184:ILE:CD1	2.48	0.41
1:C:322:TYR:O	1:C:326:MSE:HG2	2.21	0.41
1:A:118:LEU:O	1:A:119:ASP:HB3	2.21	0.41
1:B:121:ASP:CG	1:B:122:SER:H	2.26	0.41
1:B:252:LEU:HD12	1:B:252:LEU:HA	1.89	0.40
1:B:133:THR:HG22	1:B:134:ASP:N	2.35	0.40
1:B:157:VAL:HG13	1:B:216:PHE:HD1	1.87	0.40
1:B:225:PRO:HD3	1:B:251:ILE:HG12	2.02	0.40
1:B:84:ILE:HG21	1:B:111:MSE:HE1	2.02	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	A	300/313 (96%)	294 (98%)	6 (2%)	0	100	100
1	B	300/313 (96%)	283 (94%)	16 (5%)	1 (0%)	36	50
1	C	300/313 (96%)	289 (96%)	10 (3%)	1 (0%)	36	50
1	D	300/313 (96%)	289 (96%)	11 (4%)	0	100	100
All	All	1200/1252 (96%)	1155 (96%)	43 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	VAL
1	C	237	VAL

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	247/245 (101%)	240 (97%)	7 (3%)	38	60
1	B	247/245 (101%)	240 (97%)	7 (3%)	38	60
1	C	247/245 (101%)	240 (97%)	7 (3%)	38	60
1	D	247/245 (101%)	236 (96%)	11 (4%)	24	42
All	All	988/980 (101%)	956 (97%)	32 (3%)	34	56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	41	VAL
1	A	127	ARG
1	A	188	ASP
1	A	252	LEU
1	A	270	MSE
1	A	323	LEU
1	B	39	LYS
1	B	73	ILE
1	B	82	SER
1	B	188	ASP
1	B	250	ASP
1	B	252	LEU
1	B	302	LYS
1	C	39	LYS
1	C	41	VAL
1	C	43	PRO
1	C	78	GLN
1	C	146	MSE
1	C	252	LEU
1	C	270	MSE
1	D	39	LYS
1	D	62	ASP
1	D	118	LEU
1	D	127	ARG
1	D	148	GLU
1	D	181	ASP
1	D	188	ASP
1	D	252	LEU
1	D	292	MSE
1	D	302	LYS
1	D	323	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	50	GLN
1	A	74	ASN
1	A	89	ASN
1	A	173	GLN
1	A	233	ASN
1	A	266	GLN

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Mol	Chain	Res	Type
1	B	50	GLN
1	B	89	ASN
1	B	173	GLN
1	B	208	ASN
1	C	74	ASN
1	C	89	ASN
1	C	173	GLN
1	D	47	GLN
1	D	69	GLN
1	D	89	ASN
1	D	173	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	BGC	D	400	-	12,12,12	0.52	0	17,17,17	0.53	0
2	BGC	C	400	-	12,12,12	0.45	0	17,17,17	0.37	0
2	BGC	A	400	-	12,12,12	0.52	0	17,17,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	B	400	-	12,12,12	0.41	0	17,17,17	0.59	0

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	BGC	D	400	-	-	0/2/22/22	0/1/1/1
2	BGC	C	400	-	-	0/2/22/22	0/1/1/1
2	BGC	A	400	-	-	0/2/22/22	0/1/1/1
2	BGC	B	400	-	-	0/2/22/22	0/1/1/1

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 [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 ⓘ

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	A	291/313 (92%)	-0.18	3 (1%) 79 76	9, 24, 50, 67	0
1	B	291/313 (92%)	0.36	19 (6%) 25 21	8, 32, 59, 65	0
1	C	291/313 (92%)	0.29	14 (4%) 35 32	12, 35, 61, 70	0
1	D	291/313 (92%)	-0.14	2 (0%) 84 81	11, 26, 49, 57	0
All	All	1164/1252 (92%)	0.08	38 (3%) 49 45	8, 28, 58, 70	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	ILE	5.9
1	A	333	ILE	5.1
1	B	333	ILE	4.7
1	C	333	ILE	4.5
1	A	299	VAL	4.2
1	C	299	VAL	4.0
1	C	300	ASP	3.3
1	B	213	LEU	2.9
1	C	332	PRO	2.8
1	B	198	ARG	2.5
1	B	240	VAL	2.5
1	C	137	GLN	2.5
1	B	317	GLU	2.5
1	B	154	GLY	2.4
1	B	137	GLN	2.4
1	C	184	ILE	2.4
1	C	240	VAL	2.3
1	C	331	ILE	2.3
1	B	208	ASN	2.3
1	B	329	LEU	2.3
1	C	186	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	234	ALA	2.3
1	C	237	VAL	2.3
1	C	149	LEU	2.2
1	C	226	ALA	2.2
1	B	323	LEU	2.2
1	B	331	ILE	2.2
1	B	242	ILE	2.2
1	B	262	ALA	2.1
1	B	235	GLY	2.1
1	B	144	LEU	2.1
1	B	319	LEU	2.1
1	C	301	GLY	2.1
1	B	315	THR	2.1
1	B	302	LYS	2.1
1	C	210	HIS	2.1
1	B	239	LYS	2.0
1	A	300	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
2	BGC	B	400	12/12	0.93	0.08	20,22,24,27	0
2	BGC	C	400	12/12	0.95	0.07	21,25,26,27	0
2	BGC	A	400	12/12	0.96	0.06	11,15,17,18	0
2	BGC	D	400	12/12	0.96	0.06	17,19,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.