



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 06:28 PM EDT

PDB ID : 2NWW
Title : Crystal structure of GltPh in complex with TBOA
Authors : Gouaux, E.; Boudker, O.; Ryan, R.; Yernool, D.; Shimamoto, K.
Deposited on : 2006-11-16
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

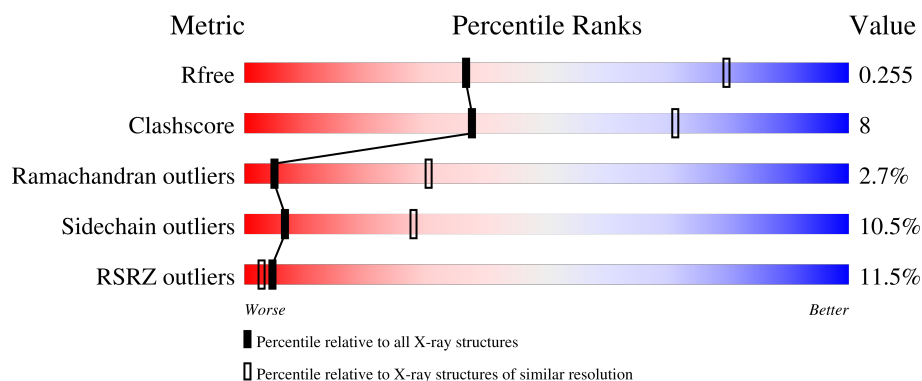
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	422	<div> <div>5%</div> <div>66%</div> <div>25%</div> <div>5%</div> <div>.</div> </div>
1	B	422	<div> <div>11%</div> <div>76%</div> <div>18%</div> <div>.</div> <div>.</div> </div>
1	C	422	<div> <div>17%</div> <div>74%</div> <div>20%</div> <div>.</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TB1	A	423	-	-	-	X
2	TB1	B	423	-	-	-	X
2	TB1	C	423	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8772 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			2906	1909	468	512	17			
1	B	407	Total	C	N	O	S	0	0	0
			2906	1909	468	512	17			
1	C	407	Total	C	N	O	S	0	0	0
			2906	1909	468	512	17			

There are 36 discrepancies between the modelled and reference sequences:

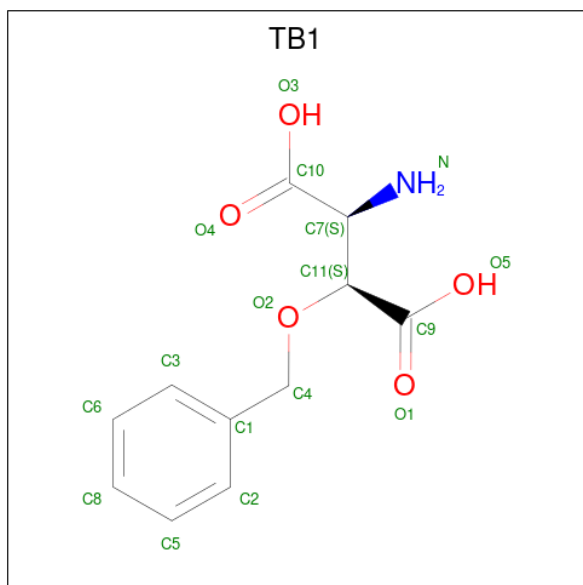
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	418	THR	-	cloning artifact	UNP O59010
A	419	LEU	-	cloning artifact	UNP O59010
A	420	VAL	-	cloning artifact	UNP O59010
A	421	PRO	-	cloning artifact	UNP O59010
A	422	ARG	-	cloning artifact	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	418	THR	-	cloning artifact	UNP O59010
B	419	LEU	-	cloning artifact	UNP O59010
B	420	VAL	-	cloning artifact	UNP O59010
B	421	PRO	-	cloning artifact	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	ARG	-	cloning artifact	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	418	THR	-	cloning artifact	UNP O59010
C	419	LEU	-	cloning artifact	UNP O59010
C	420	VAL	-	cloning artifact	UNP O59010
C	421	PRO	-	cloning artifact	UNP O59010
C	422	ARG	-	cloning artifact	UNP O59010

- Molecule 2 is (3S)-3-(BENZYLOXY)-L-ASPARTIC ACID (three-letter code: TB1) (formula: $C_{11}H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	11	1	5		
2	B	1	Total	C	N	O	0	0
			17	11	1	5		
2	C	1	Total	C	N	O	0	0
			17	11	1	5		

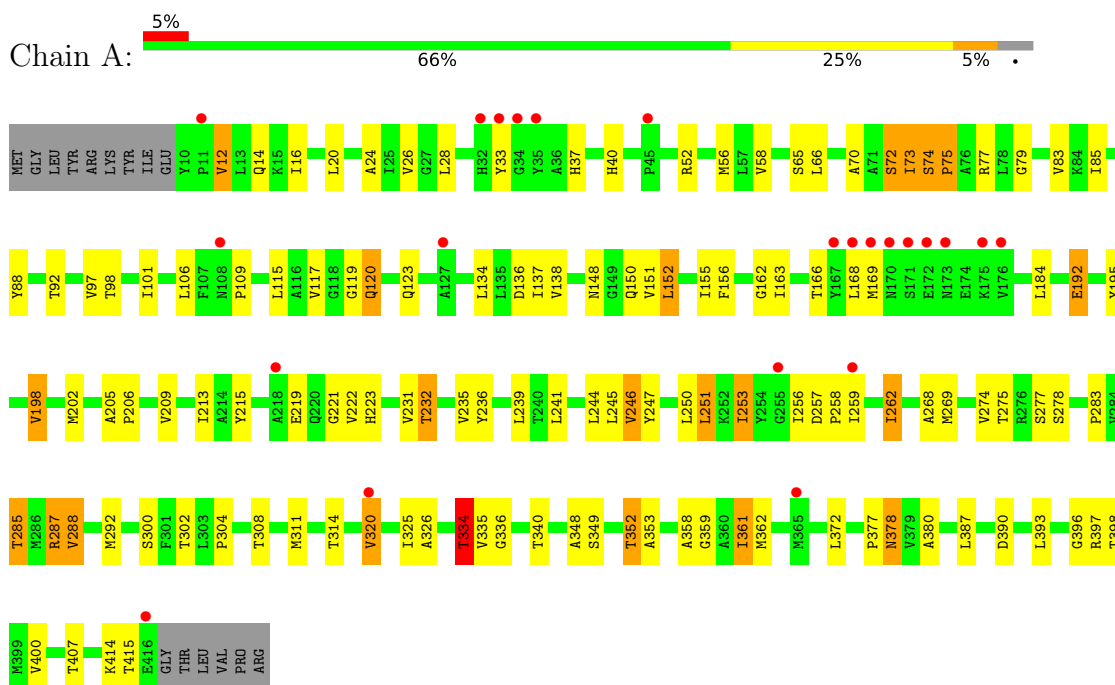
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	1	Total 1	O 1	0	0
3	C	1	Total 1	O 1	0	0

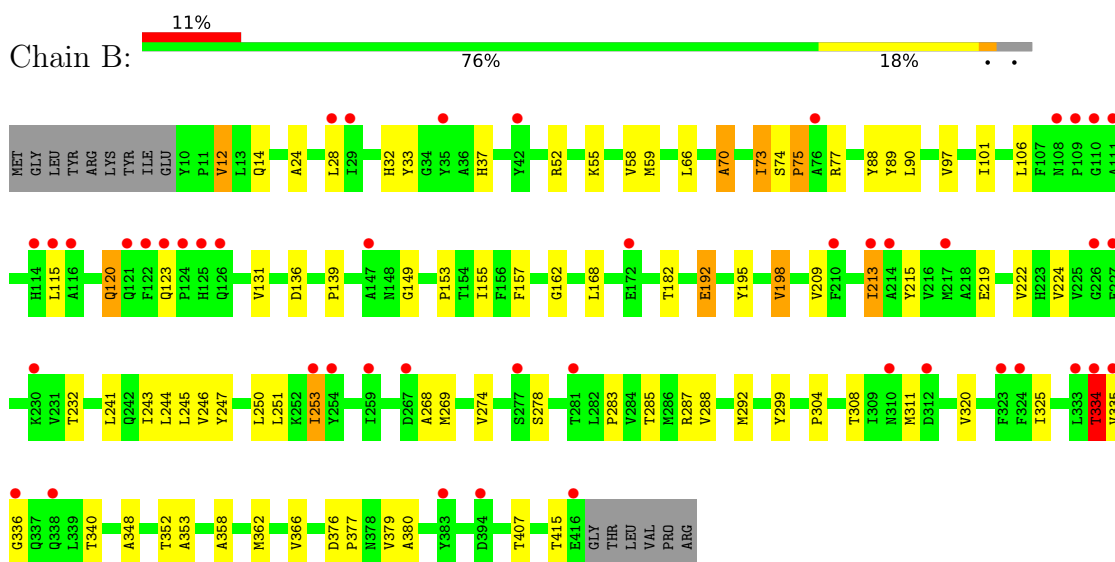
3 Residue-property plots

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 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.

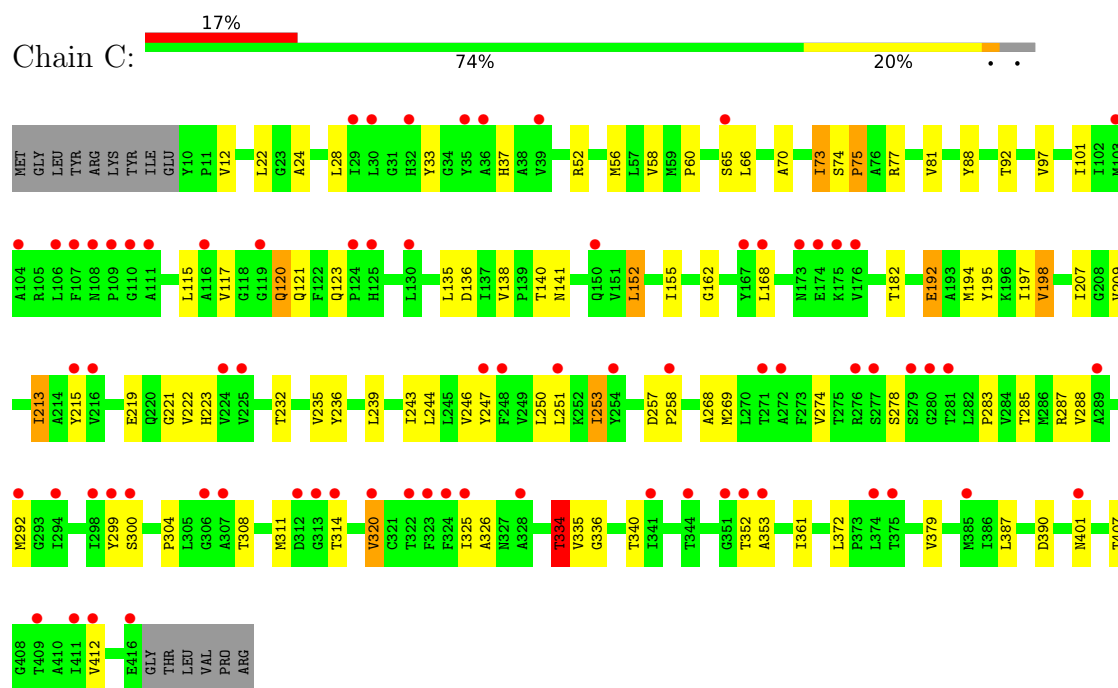
- Molecule 1: 425aa long hypothetical proton glutamate symport protein



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4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	115.25Å 115.25Å 322.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 3.20 34.17 – 3.19	Depositor EDS
% Data completeness (in resolution range)	74.8 (100.00-3.20) 74.8 (34.17-3.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.241 , 0.260 0.237 , 0.255	Depositor DCC
R_{free} test set	1516 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	135.0	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 217.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8772	wwPDB-VP
Average B, all atoms (Å ²)	201.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TB1

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	0.41	0/2961	0.62	0/4052
1	B	0.35	0/2961	0.54	0/4052
1	C	0.34	0/2961	0.53	0/4052
All	All	0.37	0/8883	0.56	0/12156

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	ALA	Peptide

5.2 Too-close contacts [i](#)

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	2906	0	2955	64	0
1	B	2906	0	2955	37	0
1	C	2906	0	2955	49	0
2	A	17	0	11	2	0
2	B	17	0	11	1	0
2	C	17	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	8772	0	8898	136	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 8.

All (136) 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:155:ILE:HD11	1:A:304:PRO:HB2	1.61	0.83
1:A:209:VAL:HG22	1:A:274:VAL:HG21	1.63	0.80
1:A:74:SER:HB2	1:A:75:PRO:HD3	1.73	0.70
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.74	0.68
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.76	0.68
1:B:192:GLU:HB3	1:C:168:LEU:HD21	1.78	0.66
1:C:387:LEU:HA	1:C:390:ASP:HB2	1.78	0.65
1:B:70:ALA:HB3	1:B:162:GLY:HA3	1.79	0.65
1:A:134:LEU:O	1:A:137:ILE:HG13	1.98	0.63
1:B:251:LEU:HD13	1:B:407:THR:HG23	1.81	0.63
1:B:52:ARG:NH2	1:C:136:ASP:HA	2.13	0.63
1:B:250:LEU:HA	1:B:253:ILE:HG22	1.82	0.62
1:C:311:MET:HB3	1:C:314:THR:HB	1.82	0.62
1:C:70:ALA:HB3	1:C:162:GLY:HA3	1.83	0.60
1:A:70:ALA:HB3	1:A:162:GLY:HA3	1.83	0.60
1:A:311:MET:HB3	1:A:314:THR:HB	1.83	0.59
1:B:209:VAL:HG22	1:B:274:VAL:HG21	1.85	0.59
1:A:195:TYR:O	1:A:198:VAL:HG12	2.03	0.59
1:B:358:ALA:HB3	2:B:423:TB1:H5	1.84	0.59
1:B:195:TYR:O	1:B:198:VAL:HG12	2.03	0.58
1:C:215:TYR:CE1	1:C:219:GLU:HG3	2.39	0.56
1:A:120:GLN:HB2	1:A:380:ALA:HB1	1.88	0.56
1:A:334:THR:O	1:A:336:GLY:N	2.40	0.55
1:A:268:ALA:HB1	1:A:285:THR:HG23	1.88	0.55
1:A:58:VAL:HG22	1:A:283:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LYS:HB3	1:C:140:THR:HG23	1.89	0.54
1:A:215:TYR:CE1	1:A:219:GLU:HG3	2.43	0.54
1:A:136:ASP:HA	1:C:52:ARG:NH2	2.21	0.54
1:B:74:SER:HB2	1:B:75:PRO:HD3	1.89	0.53
1:A:314:THR:HA	1:A:397:ARG:HD2	1.90	0.53
1:B:58:VAL:HG22	1:B:283:PRO:HD3	1.91	0.53
1:A:85:ILE:HG21	1:A:302:THR:HG22	1.91	0.52
1:A:232:THR:HA	1:A:393:LEU:HD21	1.92	0.52
1:B:334:THR:O	1:B:336:GLY:N	2.43	0.52
1:B:139:PRO:HB3	1:B:153:PRO:HB3	1.91	0.52
1:B:247:TYR:O	1:B:251:LEU:HB2	2.09	0.51
1:B:73:ILE:HB	1:B:77:ARG:HG2	1.92	0.51
1:C:209:VAL:HG22	1:C:274:VAL:HG21	1.93	0.51
1:C:195:TYR:O	1:C:198:VAL:HG12	2.10	0.51
1:B:215:TYR:CE1	1:B:219:GLU:HG3	2.46	0.51
1:C:58:VAL:HG22	1:C:283:PRO:HD3	1.93	0.51
1:A:325:ILE:HG22	1:A:372:LEU:HD13	1.93	0.51
1:B:325:ILE:HG21	1:B:379:VAL:HG13	1.92	0.51
1:B:120:GLN:HB2	1:B:380:ALA:HB1	1.93	0.50
1:C:24:ALA:O	1:C:28:LEU:HB2	2.11	0.50
1:A:250:LEU:HA	1:A:253:ILE:HG22	1.93	0.50
1:C:334:THR:O	1:C:336:GLY:N	2.44	0.50
1:A:138:VAL:O	1:C:52:ARG:NH2	2.32	0.50
1:C:268:ALA:HB1	1:C:285:THR:HG22	1.94	0.49
1:A:148:ASN:O	1:A:150:GLN:HG2	2.13	0.49
1:A:247:TYR:O	1:A:251:LEU:HB2	2.12	0.49
1:A:259:ILE:H	1:A:259:ILE:HD12	1.77	0.49
1:A:52:ARG:NH2	1:B:136:ASP:HA	2.28	0.49
1:C:236:TYR:HA	1:C:239:LEU:HD12	1.93	0.49
1:A:359:GLY:H	2:A:423:TB1:H5	1.78	0.48
1:B:24:ALA:O	1:B:28:LEU:HB2	2.12	0.48
1:A:109:PRO:HB3	1:A:231:VAL:HG22	1.96	0.48
1:C:97:VAL:O	1:C:101:ILE:HG12	2.11	0.48
1:A:239:LEU:HB3	1:A:400:VAL:HG21	1.95	0.48
1:A:348:ALA:O	1:A:352:THR:HB	2.13	0.48
1:C:221:GLY:C	1:C:223:HIS:H	2.16	0.48
1:A:202:MET:HG3	1:A:287:ARG:HH12	1.79	0.48
1:C:215:TYR:CZ	1:C:219:GLU:HG3	2.49	0.48
1:A:65:SER:O	1:A:300:SER:CB	2.62	0.47
1:A:152:LEU:HD13	1:A:308:THR:HG21	1.95	0.47
1:A:73:ILE:HB	1:A:77:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LEU:HD13	1:C:407:THR:HG23	1.96	0.47
1:A:236:TYR:CE1	1:A:396:GLY:HA3	2.49	0.47
1:A:275:THR:HG22	1:A:277:SER:HB3	1.96	0.47
1:C:325:ILE:HG21	1:C:379:VAL:HG13	1.97	0.47
1:C:401:ASN:ND2	2:C:423:TB1:O4	2.31	0.47
1:A:387:LEU:HA	1:A:390:ASP:HB2	1.96	0.46
1:B:268:ALA:HB1	1:B:285:THR:HG22	1.97	0.46
1:A:358:ALA:HA	1:A:361:ILE:HG23	1.98	0.46
1:B:149:GLY:H	1:C:141:ASN:HD22	1.62	0.46
1:C:247:TYR:O	1:C:251:LEU:HB2	2.15	0.46
1:A:209:VAL:HG13	1:A:274:VAL:HG11	1.98	0.46
1:B:243:ILE:HG22	1:B:244:LEU:HD23	1.99	0.45
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.51	0.45
1:B:288:VAL:O	1:B:292:MET:HB2	2.16	0.45
1:A:348:ALA:HB1	1:A:362:MET:HG2	1.99	0.45
1:C:243:ILE:HA	1:C:247:TYR:CD1	2.52	0.45
1:A:56:MET:CE	1:B:157:PHE:HD1	2.30	0.45
1:A:79:GLY:O	1:A:83:VAL:HG23	2.17	0.45
1:C:73:ILE:HB	1:C:77:ARG:HG2	1.98	0.45
1:A:168:LEU:HD21	1:C:192:GLU:HB3	1.98	0.45
1:A:117:VAL:HG13	1:A:377:PRO:O	2.16	0.45
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.86	0.45
1:A:262:ILE:HD13	1:A:262:ILE:HA	1.74	0.45
1:A:97:VAL:O	1:A:101:ILE:HG12	2.17	0.45
1:C:288:VAL:O	1:C:292:MET:HB2	2.17	0.44
1:A:85:ILE:HG12	1:A:302:THR:HB	1.98	0.44
1:B:88:TYR:HD2	1:B:89:TYR:CD2	2.35	0.44
1:C:251:LEU:HD23	1:C:258:PRO:HA	1.99	0.44
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.99	0.44
1:C:326:ALA:HB2	1:C:372:LEU:HD11	1.99	0.44
1:C:250:LEU:HA	1:C:253:ILE:HG22	1.98	0.44
1:C:74:SER:HB2	1:C:75:PRO:HD3	2.00	0.44
1:C:194:MET:HA	1:C:197:ILE:HD12	2.00	0.43
1:A:398:THR:HG23	2:A:423:TB1:C10	2.48	0.43
1:A:251:LEU:HD23	1:A:258:PRO:HA	2.01	0.43
1:B:213:ILE:H	1:B:213:ILE:HG13	1.64	0.43
1:A:24:ALA:O	1:A:28:LEU:HB2	2.19	0.43
1:B:376:ASP:HA	1:B:377:PRO:HD3	1.81	0.43
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.81	0.43
1:A:251:LEU:HD13	1:A:407:THR:HG23	2.00	0.43
1:A:137:ILE:HG23	1:A:152:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:C	1:A:223:HIS:H	2.22	0.43
1:A:378:ASN:HD22	1:A:378:ASN:HA	1.54	0.42
1:B:12:VAL:C	1:B:14:GLN:H	2.21	0.42
1:C:257:ASP:HA	1:C:258:PRO:HD3	1.87	0.42
1:A:40:HIS:HB2	1:A:215:TYR:HE1	1.84	0.42
1:B:97:VAL:O	1:B:101:ILE:HG12	2.19	0.42
1:B:59:MET:HG3	1:C:141:ASN:ND2	2.34	0.42
1:C:81:VAL:HG13	1:C:412:VAL:HG11	2.02	0.42
1:B:52:ARG:HG3	1:C:135:LEU:HD22	2.02	0.42
1:A:12:VAL:C	1:A:14:GLN:H	2.22	0.42
1:A:241:LEU:O	1:A:245:LEU:HB2	2.20	0.42
1:A:205:ALA:N	1:A:206:PRO:HD2	2.36	0.41
1:B:241:LEU:O	1:B:245:LEU:HB2	2.21	0.41
1:C:198:VAL:HG13	1:C:287:ARG:HD2	2.03	0.41
1:C:207:ILE:HD13	1:C:207:ILE:HA	1.87	0.41
1:A:246:VAL:O	1:A:250:LEU:HB2	2.21	0.41
1:A:288:VAL:O	1:A:292:MET:HB2	2.21	0.41
1:C:152:LEU:HD12	1:C:152:LEU:HA	1.93	0.41
1:C:213:ILE:H	1:C:213:ILE:HG13	1.71	0.41
1:A:192:GLU:HB3	1:B:168:LEU:HD21	2.02	0.41
1:B:52:ARG:NH2	1:C:138:VAL:O	2.47	0.41
1:C:60:PRO:HB2	1:C:194:MET:HG3	2.03	0.41
1:C:120:GLN:HB2	1:C:121:GLN:H	1.66	0.41
1:C:65:SER:O	1:C:300:SER:CB	2.69	0.40
1:A:326:ALA:HB2	1:A:372:LEU:HD11	2.02	0.40
1:B:348:ALA:HB1	1:B:362:MET:HG2	2.03	0.40
1:A:156:PHE:HD2	1:C:56:MET:HE3	1.85	0.40
1:C:235:VAL:HG22	1:C:320:VAL:HG11	2.03	0.40
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/422 (96%)	363 (90%)	29 (7%)	13 (3%)	4	26
1	B	405/422 (96%)	368 (91%)	27 (7%)	10 (2%)	5	32
1	C	405/422 (96%)	364 (90%)	31 (8%)	10 (2%)	5	32
All	All	1215/1266 (96%)	1095 (90%)	87 (7%)	33 (3%)	5	30

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	THR
1	A	335	VAL
1	A	353	ALA
1	B	73	ILE
1	B	334	THR
1	B	335	VAL
1	B	353	ALA
1	C	12	VAL
1	C	335	VAL
1	A	12	VAL
1	A	73	ILE
1	A	222	VAL
1	B	12	VAL
1	B	66	LEU
1	C	73	ILE
1	C	334	THR
1	A	66	LEU
1	A	72	SER
1	A	115	LEU
1	B	75	PRO
1	B	115	LEU
1	B	222	VAL
1	C	66	LEU
1	C	115	LEU
1	C	222	VAL
1	C	353	ALA
1	A	75	PRO
1	A	123	GLN
1	B	123	GLN
1	C	75	PRO
1	C	123	GLN
1	A	74	SER
1	A	119	GLY

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	283/330 (86%)	244 (86%)	39 (14%)	3	16
1	B	283/330 (86%)	256 (90%)	27 (10%)	8	32
1	C	283/330 (86%)	260 (92%)	23 (8%)	11	42
All	All	849/990 (86%)	760 (90%)	89 (10%)	7	28

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	20	LEU
1	A	26	VAL
1	A	33	TYR
1	A	37	HIS
1	A	72	SER
1	A	98	THR
1	A	106	LEU
1	A	120	GLN
1	A	151	VAL
1	A	152	LEU
1	A	163	ILE
1	A	166	THR
1	A	169	MET
1	A	184	LEU
1	A	192	GLU
1	A	198	VAL
1	A	213	ILE
1	A	232	THR
1	A	244	LEU
1	A	246	VAL
1	A	251	LEU
1	A	253	ILE
1	A	256	ILE
1	A	262	ILE
1	A	269	MET

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Mol	Chain	Res	Type
1	A	278	SER
1	A	285	THR
1	A	287	ARG
1	A	288	VAL
1	A	320	VAL
1	A	334	THR
1	A	340	THR
1	A	349	SER
1	A	352	THR
1	A	361	ILE
1	A	378	ASN
1	A	414	LYS
1	A	415	THR
1	B	32	HIS
1	B	33	TYR
1	B	37	HIS
1	B	90	LEU
1	B	106	LEU
1	B	120	GLN
1	B	131	VAL
1	B	182	THR
1	B	192	GLU
1	B	198	VAL
1	B	213	ILE
1	B	224	VAL
1	B	232	THR
1	B	246	VAL
1	B	253	ILE
1	B	269	MET
1	B	278	SER
1	B	287	ARG
1	B	299	TYR
1	B	308	THR
1	B	311	MET
1	B	320	VAL
1	B	334	THR
1	B	340	THR
1	B	352	THR
1	B	366	VAL
1	B	415	THR
1	C	22	LEU
1	C	33	TYR

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Mol	Chain	Res	Type
1	C	37	HIS
1	C	117	VAL
1	C	120	GLN
1	C	152	LEU
1	C	182	THR
1	C	192	GLU
1	C	198	VAL
1	C	213	ILE
1	C	232	THR
1	C	244	LEU
1	C	246	VAL
1	C	253	ILE
1	C	269	MET
1	C	278	SER
1	C	299	TYR
1	C	308	THR
1	C	320	VAL
1	C	334	THR
1	C	340	THR
1	C	352	THR
1	C	361	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	318	GLN
1	A	378	ASN
1	B	40	HIS
1	B	378	ASN
1	C	40	HIS
1	C	203	GLN
1	C	378	ASN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	TB1	B	423	-	10,17,17	1.63	1 (10%)	11,22,22	1.66	1 (9%)
2	TB1	A	423	-	10,17,17	1.61	2 (20%)	11,22,22	1.79	1 (9%)
2	TB1	C	423	-	10,17,17	1.60	1 (10%)	11,22,22	1.76	1 (9%)

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	TB1	B	423	-	-	7/9/17/17	0/1/1/1
2	TB1	A	423	-	-	6/9/17/17	0/1/1/1
2	TB1	C	423	-	-	6/9/17/17	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	423	TB1	C4-C1	-4.72	1.39	1.50
2	B	423	TB1	C4-C1	-4.43	1.40	1.50
2	A	423	TB1	C4-C1	-3.82	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	423	TB1	O2-C11	2.57	1.46	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	423	TB1	O2-C4-C1	5.68	122.98	109.91
2	C	423	TB1	O2-C4-C1	5.64	122.89	109.91
2	B	423	TB1	O2-C4-C1	5.28	122.08	109.91

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	423	TB1	C7-C11-O2-C4
2	A	423	TB1	O2-C11-C7-C10
2	A	423	TB1	O2-C11-C7-N
2	A	423	TB1	C9-C11-C7-C10
2	A	423	TB1	C9-C11-C7-N
2	B	423	TB1	C7-C11-O2-C4
2	B	423	TB1	O2-C11-C7-C10
2	B	423	TB1	O2-C11-C7-N
2	B	423	TB1	C9-C11-C7-C10
2	B	423	TB1	C9-C11-C7-N
2	C	423	TB1	C7-C11-O2-C4
2	C	423	TB1	O2-C11-C7-C10
2	C	423	TB1	C9-C11-C7-C10
2	B	423	TB1	C9-C11-O2-C4
2	C	423	TB1	C9-C11-O2-C4
2	C	423	TB1	C1-C4-O2-C11
2	A	423	TB1	C9-C11-O2-C4
2	C	423	TB1	O2-C11-C7-N
2	B	423	TB1	C1-C4-O2-C11

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	423	TB1	1	0
2	A	423	TB1	2	0
2	C	423	TB1	1	0

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	A	407/422 (96%)	0.29	23 (5%) 23 13	162, 192, 224, 262	0
1	B	407/422 (96%)	0.54	45 (11%) 5 3	158, 202, 229, 263	0
1	C	407/422 (96%)	0.77	73 (17%) 1 1	163, 204, 237, 274	0
All	All	1221/1266 (96%)	0.53	141 (11%) 4 3	158, 199, 231, 274	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	GLY	8.9
1	B	124	PRO	8.8
1	B	122	PHE	8.2
1	B	123	GLN	7.2
1	C	109	PRO	6.8
1	B	108	ASN	6.8
1	C	110	GLY	6.1
1	A	33	TYR	6.1
1	B	109	PRO	6.1
1	C	176	VAL	5.9
1	C	324	PHE	5.6
1	C	124	PRO	5.5
1	A	35	TYR	5.4
1	B	111	ALA	5.4
1	B	210	PHE	5.3
1	A	169	MET	5.1
1	A	170	ASN	5.0
1	B	226	GLY	4.9
1	B	227	GLU	4.8
1	B	267	ASP	4.7
1	B	335	VAL	4.7
1	B	333	LEU	4.6
1	B	35	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	11	PRO	4.6
1	A	171	SER	4.5
1	C	281	THR	4.5
1	C	325	ILE	4.4
1	C	215	TYR	4.4
1	B	76	ALA	4.3
1	C	248	PHE	4.2
1	C	314	THR	4.2
1	B	121	GLN	4.2
1	C	107	PHE	4.1
1	A	168	LEU	4.1
1	C	225	VAL	4.0
1	A	176	VAL	4.0
1	C	175	LYS	4.0
1	B	114	HIS	3.9
1	C	29	ILE	3.9
1	C	323	PHE	3.8
1	C	111	ALA	3.7
1	C	344	THR	3.7
1	C	277	SER	3.7
1	C	401	ASN	3.7
1	C	35	TYR	3.6
1	C	104	ALA	3.6
1	C	280	GLY	3.6
1	B	253	ILE	3.6
1	B	110	GLY	3.5
1	C	254	TYR	3.4
1	C	313	GLY	3.4
1	A	365	MET	3.4
1	C	279	SER	3.4
1	C	294	ILE	3.3
1	B	214	ALA	3.3
1	C	374	LEU	3.3
1	C	353	ALA	3.3
1	B	125	HIS	3.3
1	C	108	ASN	3.2
1	C	312	ASP	3.2
1	C	36	ALA	3.2
1	B	338	GLN	3.1
1	B	29	ILE	3.1
1	C	292	MET	3.1
1	B	28	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLY	3.0
1	C	106	LEU	3.0
1	C	173	ASN	3.0
1	C	167	TYR	3.0
1	B	334	THR	2.9
1	B	394	ASP	2.9
1	B	213	ILE	2.9
1	A	173	ASN	2.9
1	A	172	GLU	2.9
1	B	230	LYS	2.9
1	B	126	GLN	2.9
1	C	271	THR	2.8
1	C	375	THR	2.8
1	C	65	SER	2.8
1	A	108	ASN	2.8
1	C	272	ALA	2.8
1	B	147	ALA	2.8
1	C	247	TYR	2.7
1	B	259	ILE	2.7
1	B	116	ALA	2.7
1	C	224	VAL	2.7
1	B	310	ASN	2.7
1	C	174	GLU	2.7
1	C	352	THR	2.7
1	C	385	MET	2.6
1	C	412	VAL	2.6
1	C	411	ILE	2.6
1	C	168	LEU	2.6
1	B	323	PHE	2.6
1	B	217	MET	2.6
1	C	103	MET	2.6
1	B	42	TYR	2.6
1	C	276	ARG	2.6
1	C	289	ALA	2.5
1	A	32	HIS	2.5
1	C	322	THR	2.5
1	A	416	GLU	2.5
1	B	254	TYR	2.5
1	A	167	TYR	2.4
1	B	383	TYR	2.4
1	C	328	ALA	2.4
1	A	34	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	32	HIS	2.4
1	C	299	TYR	2.4
1	C	416	GLU	2.3
1	B	115	LEU	2.3
1	C	307	ALA	2.3
1	C	251	LEU	2.3
1	A	259	ILE	2.3
1	B	324	PHE	2.3
1	C	119	GLY	2.3
1	C	351	GLY	2.2
1	C	30	LEU	2.2
1	A	175	LYS	2.2
1	C	150	GLN	2.2
1	C	39	VAL	2.2
1	B	416	GLU	2.2
1	A	127	ALA	2.1
1	C	300	SER	2.1
1	C	116	ALA	2.1
1	C	306	GLY	2.1
1	B	277	SER	2.1
1	B	312	ASP	2.1
1	C	320	VAL	2.1
1	C	409	THR	2.1
1	C	130	LEU	2.1
1	C	258	PRO	2.1
1	A	218	ALA	2.1
1	B	281	THR	2.1
1	A	45	PRO	2.1
1	C	298	ILE	2.1
1	A	320	VAL	2.0
1	C	216	VAL	2.0
1	C	341	ILE	2.0
1	B	172	GLU	2.0
1	C	125	HIS	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 [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	TB1	C	423	17/17	0.46	1.00	203,208,210,211	0
2	TB1	A	423	17/17	0.58	1.26	179,185,198,198	0
2	TB1	B	423	17/17	0.69	1.08	237,242,252,252	0

6.5 Other polymers [i](#)

There are no such residues in this entry.