Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 03:42 AM EDT

PDB ID	:	3FZ0
Title	:	Inosine-Guanosine Nucleoside Hydrolase (IG-NH)
Authors	:	Vandemeulebroucke, A.; Minici, C.; Bruno, I.; Muzzolini, L.; Tornaghi, P.; Parkin, D.W.; Schramm, V.L.; Versees, W.; Steyaert, J.; Degano, M.
Deposited on	:	2009-01-23
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

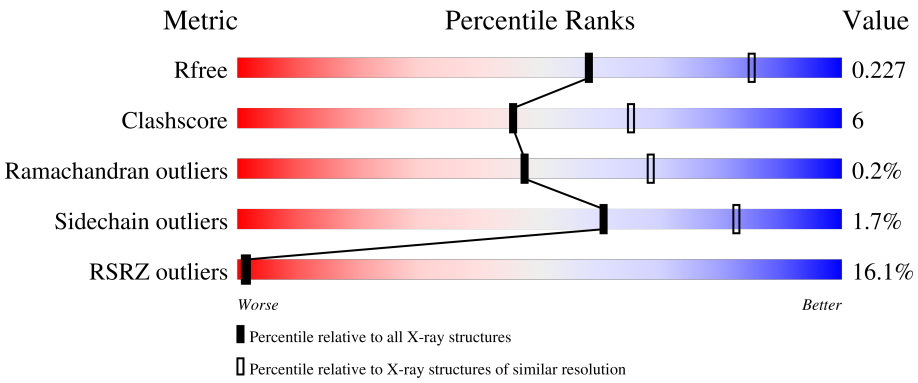
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	360	13% 78% 12% 9%
1	B	360	11% 80% 13% • 6%
1	C	360	15% 79% 12% 9%
1	D	360	19% 77% 12% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10597 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 Nucleoside hydrolase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2568	1635	436	483	14	0	3	0
1	B	338	2648	1682	454	498	14	0	3	0
1	C	328	2580	1641	439	486	14	0	4	0
1	D	326	2555	1626	435	480	14	0	2	0

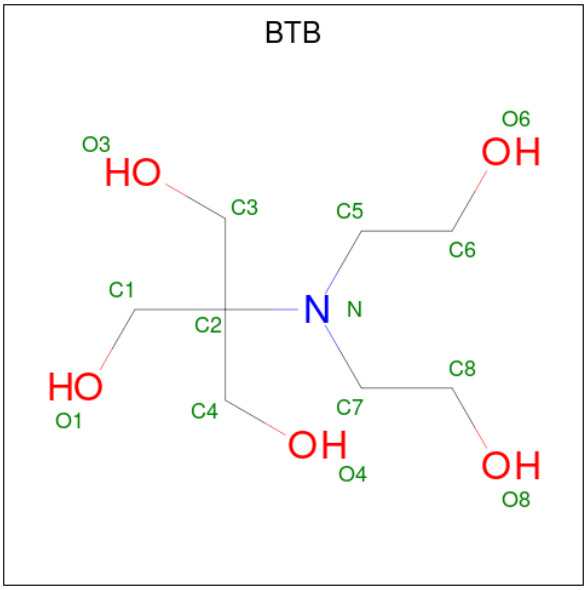
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q57X73
A	-1	SER	-	expression tag	UNP Q57X73
A	0	HIS	-	expression tag	UNP Q57X73
A	97	GLN	LYS	engineered mutation	UNP Q57X73
A	226	SER	LEU	engineered mutation	UNP Q57X73
B	-2	GLY	-	expression tag	UNP Q57X73
B	-1	SER	-	expression tag	UNP Q57X73
B	0	HIS	-	expression tag	UNP Q57X73
B	97	GLN	LYS	engineered mutation	UNP Q57X73
B	226	SER	LEU	engineered mutation	UNP Q57X73
C	-2	GLY	-	expression tag	UNP Q57X73
C	-1	SER	-	expression tag	UNP Q57X73
C	0	HIS	-	expression tag	UNP Q57X73
C	97	GLN	LYS	engineered mutation	UNP Q57X73
C	226	SER	LEU	engineered mutation	UNP Q57X73
D	-2	GLY	-	expression tag	UNP Q57X73
D	-1	SER	-	expression tag	UNP Q57X73
D	0	HIS	-	expression tag	UNP Q57X73
D	97	GLN	LYS	engineered mutation	UNP Q57X73
D	226	SER	LEU	engineered mutation	UNP Q57X73

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is water.

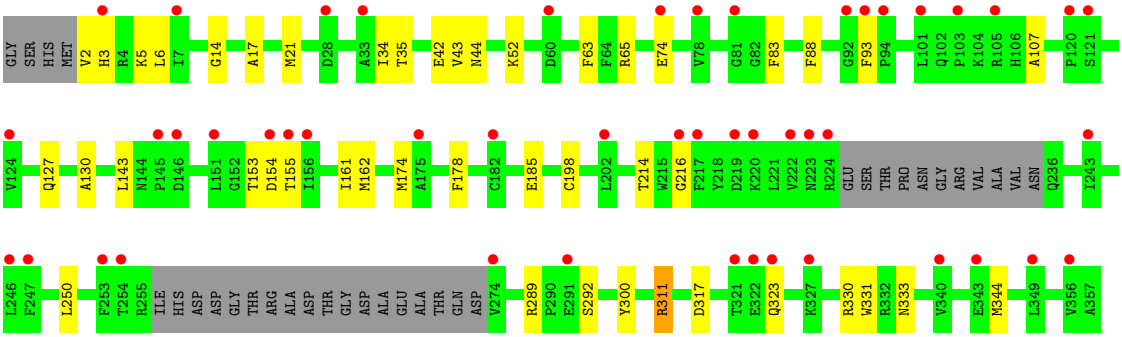
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	46	46	46	0	0
			Total	O		
4	B	55	55	55	0	0
			Total	O		
4	C	55	55	55	0	0
			Total	O		
4	D	30	30	30	0	0

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.

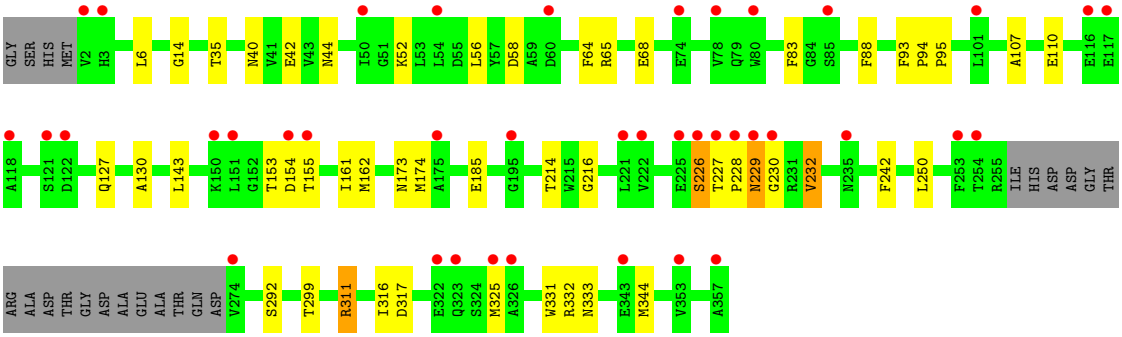
• Molecule 1: Nucleoside hydrolase, putative

Chain A:



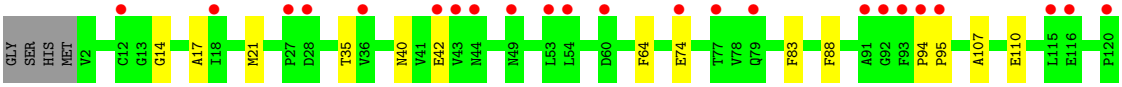
• Molecule 1: Nucleoside hydrolase, putative

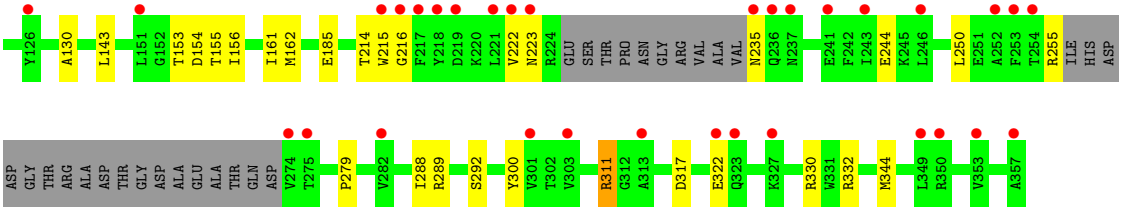
Chain B:



• Molecule 1: Nucleoside hydrolase, putative

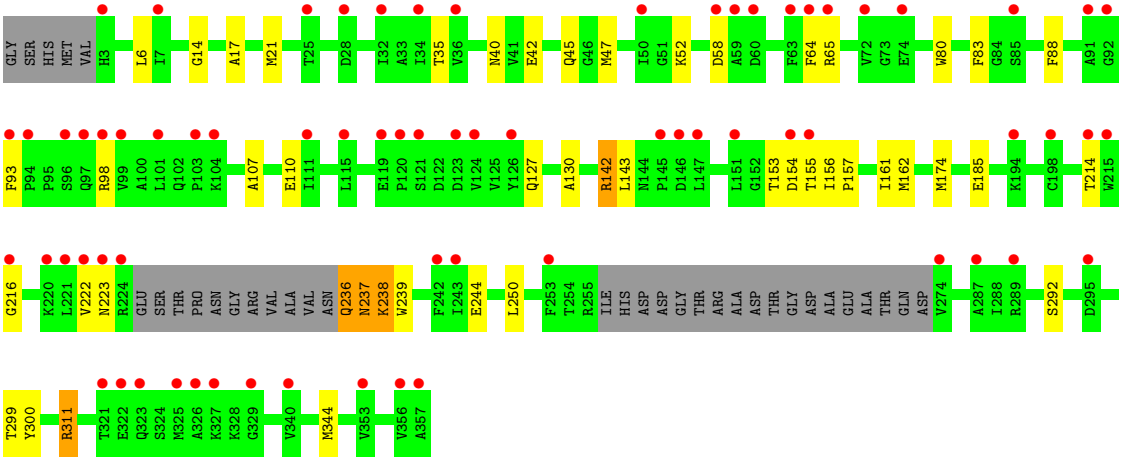
Chain C:





- Molecule 1: Nucleoside hydrolase, putative

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	124.69Å 116.04Å 204.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.50 19.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.93-2.50) 99.9 (19.93-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	4.02 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.224 0.192 , 0.227	Depositor DCC
R_{free} test set	2620 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10597	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BTB, 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	A	0.71	1/2629 (0.0%)	0.70	1/3572 (0.0%)
1	B	0.73	0/2712	0.75	2/3688 (0.1%)
1	C	0.73	5/2644 (0.2%)	0.72	2/3593 (0.1%)
1	D	0.68	4/2613 (0.2%)	0.72	3/3550 (0.1%)
All	All	0.71	10/10598 (0.1%)	0.72	8/14403 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	GLN	CB-CG	8.67	1.75	1.52
1	D	238	LYS	C-O	8.64	1.39	1.23
1	C	235	ASN	CG-ND2	8.05	1.52	1.32
1	C	235	ASN	CG-OD1	6.65	1.38	1.24
1	A	198	CYS	CB-SG	-5.80	1.72	1.81
1	D	238	LYS	CE-NZ	5.47	1.62	1.49
1	C	42	GLU	CG-CD	5.18	1.59	1.51
1	C	322	GLU	CG-CD	5.02	1.59	1.51
1	C	74	GLU	CG-CD	5.01	1.59	1.51
1	D	237	ASN	CB-CG	5.01	1.62	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	311	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	B	311	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	311	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	311	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	332	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	311	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	311	ARG	NE-CZ-NH1	5.28	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	142	ARG	NE-CZ-NH2	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2568	0	2549	29	0
1	B	2648	0	2627	40	0
1	C	2580	0	2559	28	0
1	D	2555	0	2534	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	14	0	19	3	0
3	B	14	0	19	3	0
3	C	14	0	19	5	0
3	D	14	0	19	3	0
4	A	46	0	0	0	0
4	B	55	0	0	4	0
4	C	55	0	0	0	0
4	D	30	0	0	0	0
All	All	10597	0	10345	132	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 6.

All (132) 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:D:236:GLN:CB	1:D:236:GLN:CG	1.76	1.62
1:B:143:LEU:HD11	1:D:143:LEU:HD11	1.27	1.15
1:B:226:SER:HA	1:B:227:THR:C	1.82	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASN:HB2	4:B:364:HOH:O	1.64	0.95
1:A:143:LEU:HD11	1:C:143:LEU:HD11	1.51	0.91
1:C:214:THR:HG22	1:C:216:GLY:H	1.44	0.82
1:D:214:THR:HG22	1:D:216:GLY:H	1.46	0.78
1:B:214:THR:HG22	1:B:216:GLY:H	1.49	0.78
3:C:401:BTB:H82	3:C:401:BTB:O6	1.83	0.77
1:B:65[B]:ARG:NH2	1:B:68:GLU:OE2	2.19	0.75
1:C:40:ASN:HD21	3:C:401:BTB:H61	1.50	0.74
3:B:401:BTB:H82	3:B:401:BTB:C6	2.19	0.72
1:D:292:SER:HB3	1:D:344:MET:HE1	1.71	0.72
1:B:44:ASN:OD1	1:B:65[B]:ARG:NH1	2.23	0.72
1:C:292:SER:HB3	1:C:344:MET:HE2	1.71	0.72
1:B:292:SER:HB3	1:B:344:MET:HE1	1.72	0.71
1:B:214:THR:HG22	1:B:216:GLY:N	2.06	0.69
1:D:214:THR:HG22	1:D:216:GLY:N	2.06	0.69
1:C:214:THR:HG22	1:C:216:GLY:N	2.08	0.69
1:A:214:THR:HG22	1:A:216:GLY:H	1.58	0.68
1:B:83:PHE:HD1	4:B:411:HOH:O	1.78	0.66
1:A:292:SER:HB3	1:A:344:MET:HE1	1.76	0.66
1:D:236:GLN:CB	1:D:236:GLN:CD	2.65	0.65
1:B:226:SER:OG	1:B:229:ASN:HA	1.95	0.65
1:A:153:THR:HG22	1:A:154:ASP:N	2.12	0.64
1:A:214:THR:HG22	1:A:216:GLY:N	2.13	0.63
1:D:47:MET:HG3	1:D:65:ARG:NH1	2.14	0.62
1:B:228:PRO:HA	1:B:229:ASN:HB3	1.79	0.62
1:C:153:THR:HG22	1:C:154:ASP:N	2.16	0.61
1:A:153:THR:HG22	1:A:155:THR:H	1.66	0.60
1:A:3:HIS:CD2	1:A:5:LYS:HZ3	2.20	0.59
1:D:236:GLN:CG	1:D:236:GLN:CA	2.76	0.59
1:A:44:ASN:OD1	1:A:65[B]:ARG:NH1	2.36	0.58
1:C:185:GLU:OE2	1:C:311:ARG:NH2	2.34	0.58
1:C:222:VAL:HG11	1:C:244:GLU:HB2	1.87	0.57
1:A:185:GLU:OE2	1:A:311:ARG:NH2	2.37	0.56
1:B:153:THR:HG22	1:B:154:ASP:N	2.21	0.56
1:B:35:THR:HB	1:B:107:ALA:HB1	1.89	0.55
1:D:153:THR:HG22	1:D:154:ASP:N	2.21	0.55
1:C:222:VAL:CG1	1:C:244:GLU:HB2	2.37	0.54
1:B:230:GLY:O	1:B:232:VAL:HG22	2.08	0.54
1:B:153:THR:HG22	1:B:155:THR:H	1.73	0.53
1:C:14:GLY:HA3	1:C:83:PHE:CE2	2.43	0.53
1:C:130:ALA:HB3	1:C:161:ILE:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:401:BTB:H82	3:B:401:BTB:H61	1.90	0.53
1:A:185:GLU:CD	1:A:311:ARG:HH22	2.12	0.53
1:A:153:THR:CG2	1:A:154:ASP:N	2.72	0.52
1:C:40:ASN:HD21	3:C:401:BTB:C6	2.20	0.52
1:C:153:THR:HG22	1:C:154:ASP:OD1	2.10	0.52
1:B:14:GLY:HA3	1:B:83:PHE:CE2	2.45	0.51
1:D:185:GLU:OE2	1:D:311:ARG:NH2	2.38	0.51
1:B:6:LEU:HD22	1:B:127:GLN:HB2	1.94	0.50
1:B:143:LEU:CD1	1:D:143:LEU:HD11	2.20	0.50
1:C:153:THR:HG22	1:C:155:THR:H	1.77	0.50
1:B:153:THR:HG22	1:B:154:ASP:OD1	2.12	0.50
1:D:153:THR:HG22	1:D:155:THR:H	1.78	0.49
1:C:300:TYR:CD2	1:C:330:ARG:HD3	2.48	0.49
1:B:226:SER:CA	1:B:227:THR:C	2.71	0.48
1:D:153:THR:HG22	1:D:154:ASP:OD1	2.13	0.48
1:B:331:TRP:CE2	1:B:333:ASN:HB3	2.49	0.48
1:C:14:GLY:HA3	1:C:83:PHE:CD2	2.49	0.48
1:D:17:ALA:O	1:D:21:MET:HG3	2.13	0.48
1:A:153:THR:HG22	1:A:154:ASP:OD1	2.14	0.48
1:D:185:GLU:CD	1:D:311:ARG:HH22	2.15	0.47
1:B:228:PRO:CA	1:B:229:ASN:HB3	2.44	0.47
1:D:58:ASP:OD1	1:D:98:ARG:NH2	2.46	0.47
1:A:289:ARG:HH11	1:A:344:MET:HE2	1.78	0.47
1:A:52:LYS:HD3	1:A:93:PHE:HB2	1.96	0.47
1:D:42[B]:GLU:HG2	1:D:45:GLN:H	1.79	0.47
1:D:52:LYS:HD3	1:D:93:PHE:HB2	1.97	0.47
1:C:153:THR:CG2	1:C:154:ASP:N	2.78	0.47
1:D:130:ALA:HB3	1:D:161:ILE:HG22	1.97	0.47
1:B:185:GLU:OE2	1:B:311:ARG:NH2	2.41	0.46
1:D:35:THR:HB	1:D:107:ALA:HB1	1.96	0.46
1:D:14:GLY:HA3	1:D:83:PHE:CE2	2.50	0.46
3:A:401:BTB:H52	3:A:401:BTB:H81	1.70	0.46
1:B:185:GLU:CD	1:B:311:ARG:HH22	2.17	0.46
1:A:35:THR:HB	1:A:107:ALA:HB1	1.97	0.46
1:D:237:ASN:OD1	1:D:239:TRP:N	2.40	0.46
1:D:40:ASN:HD21	3:D:401:BTB:C3	2.29	0.45
1:A:178:PHE:HB3	3:A:401:BTB:H11	1.99	0.45
1:C:289:ARG:HH11	1:C:344:MET:HE3	1.82	0.45
3:A:401:BTB:H51	3:A:401:BTB:H42	1.47	0.45
3:B:401:BTB:H32	4:B:372:HOH:O	2.16	0.45
1:A:130:ALA:HB3	1:A:161:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:THR:HB	1:D:156:ILE:H	1.82	0.45
1:C:185:GLU:CD	1:C:311:ARG:HH22	2.19	0.44
1:A:331:TRP:CE2	1:A:333:ASN:HB3	2.51	0.44
1:B:153:THR:CG2	1:B:154:ASP:N	2.80	0.44
3:D:401:BTB:H72	3:D:401:BTB:H61	1.59	0.44
1:A:300:TYR:CD2	1:A:330:ARG:HD3	2.52	0.44
1:D:6:LEU:HD22	1:D:127:GLN:HB2	2.00	0.44
1:C:35:THR:HB	1:C:107:ALA:HB1	1.99	0.44
1:A:17:ALA:O	1:A:21:MET:HG3	2.18	0.44
1:A:174:MET:HE3	1:B:317:ASP:HB2	2.00	0.43
1:D:64:PHE:CD1	1:D:110:GLU:HG2	2.53	0.43
1:B:64:PHE:CD1	1:B:110:GLU:HG2	2.53	0.43
1:D:222:VAL:CG1	1:D:244:GLU:HB2	2.48	0.43
1:A:14:GLY:HA3	1:A:83:PHE:CE2	2.54	0.43
1:C:279:PRO:HG2	3:C:401:BTB:H31	2.00	0.42
1:D:80:TRP:CG	3:D:401:BTB:H82	2.54	0.42
1:A:83:PHE:CZ	1:A:250:LEU:HD22	2.54	0.42
1:A:317:ASP:HB2	1:B:174:MET:HE3	2.01	0.42
1:C:317:ASP:HB2	1:D:174:MET:HE3	2.01	0.42
1:B:94:PRO:HA	1:B:95:PRO:HD3	1.97	0.42
1:A:43:VAL:CG1	1:A:65[A]:ARG:HG2	2.49	0.42
1:B:226:SER:HA	1:B:227:THR:O	2.15	0.42
1:D:156:ILE:HA	1:D:157:PRO:HD3	1.95	0.42
1:D:153:THR:CG2	1:D:154:ASP:N	2.83	0.42
3:C:401:BTB:H12	3:C:401:BTB:H72	1.64	0.41
1:B:83:PHE:CZ	1:B:250:LEU:HD22	2.55	0.41
1:B:173:ASN:HB2	4:B:363:HOH:O	2.20	0.41
1:A:153:THR:CG2	1:A:154:ASP:H	2.33	0.41
1:B:130:ALA:HB3	1:B:161:ILE:HG22	2.02	0.41
1:C:153:THR:HB	1:C:156:ILE:H	1.86	0.41
1:B:56:LEU:HD22	1:B:242:PHE:CG	2.55	0.41
1:C:64:PHE:CD1	1:C:110:GLU:HG2	2.55	0.41
1:C:215:TRP:HB3	1:C:255:ARG:CZ	2.50	0.41
1:D:299:THR:OG1	1:D:300:TYR:N	2.54	0.41
1:A:174:MET:HE2	1:B:316:ILE:C	2.40	0.41
1:B:14:GLY:HA3	1:B:83:PHE:CD2	2.55	0.41
1:B:229:ASN:HA	1:B:230:GLY:HA2	1.90	0.41
1:A:6:LEU:HD22	1:A:127:GLN:HB2	2.02	0.41
1:B:325:MET:HB2	1:B:325:MET:HE2	1.81	0.41
1:B:299:THR:HA	1:B:332:ARG:HG2	2.02	0.41
1:C:83:PHE:CZ	1:C:250:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:PRO:HA	1:C:95:PRO:HD3	1.97	0.40
1:C:17:ALA:O	1:C:21:MET:HG3	2.21	0.40
1:D:83:PHE:CZ	1:D:250:LEU:HD22	2.56	0.40
1:D:142:ARG:HH11	1:D:142:ARG:HA	1.85	0.40
1:B:52:LYS:HD3	1:B:93:PHE:HB2	2.03	0.40
1:A:34:ILE:O	1:A:63:PHE:HA	2.21	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	324/360 (90%)	316 (98%)	8 (2%)	0	100	100
1	B	337/360 (94%)	321 (95%)	14 (4%)	2 (1%)	25	43
1	C	326/360 (91%)	316 (97%)	10 (3%)	0	100	100
1	D	322/360 (89%)	311 (97%)	11 (3%)	0	100	100
All	All	1309/1440 (91%)	1264 (97%)	43 (3%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	226	SER
1	B	229	ASN

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	279/301 (93%)	271 (97%)	8 (3%)	42	69
1	B	288/301 (96%)	283 (98%)	5 (2%)	60	82
1	C	281/301 (93%)	277 (99%)	4 (1%)	67	86
1	D	277/301 (92%)	273 (99%)	4 (1%)	67	86
All	All	1125/1204 (93%)	1104 (98%)	21 (2%)	60	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	42[A]	GLU
1	A	42[B]	GLU
1	A	74[A]	GLU
1	A	74[B]	GLU
1	A	88	PHE
1	A	162	MET
1	A	323	GLN
1	B	42	GLU
1	B	58	ASP
1	B	88	PHE
1	B	162	MET
1	B	232	VAL
1	C	88	PHE
1	C	162	MET
1	C	223	ASN
1	C	288	ILE
1	D	88	PHE
1	D	162	MET
1	D	223	ASN
1	D	238	LYS

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

Mol	Chain	Res	Type
1	C	40	ASN
1	D	40	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	BTB	B	401	-	13,13,13	0.45	0	7,16,16	1.19	0
3	BTB	D	401	-	13,13,13	0.40	0	7,16,16	0.48	0
3	BTB	C	401	-	13,13,13	0.44	0	7,16,16	0.45	0
3	BTB	A	401	-	13,13,13	0.51	0	7,16,16	1.15	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
3	BTB	B	401	-	-	8/21/21/21	-
3	BTB	D	401	-	-	9/21/21/21	-
3	BTB	C	401	-	-	6/21/21/21	-
3	BTB	A	401	-	-	11/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	BTB	C1-C2-C3-O3
3	A	401	BTB	C4-C2-C3-O3
3	A	401	BTB	N-C2-C3-O3
3	A	401	BTB	C1-C2-C4-O4
3	A	401	BTB	C3-C2-C4-O4
3	A	401	BTB	N-C2-C4-O4
3	A	401	BTB	C3-C2-N-C5
3	A	401	BTB	C4-C2-N-C5
3	A	401	BTB	C8-C7-N-C5
3	B	401	BTB	C1-C2-C4-O4
3	B	401	BTB	C3-C2-C4-O4
3	B	401	BTB	N-C2-C4-O4
3	B	401	BTB	C1-C2-N-C7
3	B	401	BTB	C4-C2-N-C7
3	B	401	BTB	C8-C7-N-C5
3	B	401	BTB	N-C5-C6-O6
3	C	401	BTB	C1-C2-N-C7
3	C	401	BTB	C4-C2-N-C7
3	D	401	BTB	C1-C2-C4-O4
3	D	401	BTB	C3-C2-C4-O4
3	D	401	BTB	N-C2-C4-O4
3	D	401	BTB	C1-C2-N-C7
3	D	401	BTB	C3-C2-N-C7
3	D	401	BTB	C4-C2-N-C7
3	D	401	BTB	C6-C5-N-C7
3	D	401	BTB	N-C7-C8-O8
3	C	401	BTB	N-C7-C8-O8
3	D	401	BTB	N-C5-C6-O6
3	C	401	BTB	C1-C2-C4-O4
3	A	401	BTB	C1-C2-N-C5
3	B	401	BTB	C3-C2-N-C7
3	C	401	BTB	C3-C2-N-C7
3	A	401	BTB	N-C7-C8-O8
3	C	401	BTB	C3-C2-C4-O4

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	BTB	3	0
3	D	401	BTB	3	0
3	C	401	BTB	5	0
3	A	401	BTB	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	327/360 (90%)	1.01	48 (14%)	2	2	56, 63, 71, 79	0
1	B	338/360 (93%)	0.91	40 (11%)	4	4	57, 63, 73, 86	0
1	C	328/360 (91%)	1.09	55 (16%)	1	1	57, 63, 71, 79	0
1	D	326/360 (90%)	1.29	70 (21%)	0	0	57, 63, 71, 79	0
All	All	1319/1440 (91%)	1.07	213 (16%)	1	1	56, 63, 72, 86	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	274	VAL	10.0
1	B	227	THR	8.8
1	C	252	ALA	7.9
1	B	228	PRO	7.3
1	A	274	VAL	6.9
1	B	154	ASP	6.7
1	B	122	ASP	6.5
1	D	321	THR	6.4
1	D	94	PRO	5.6
1	D	146	ASP	5.6
1	D	97	GLN	5.6
1	D	274	VAL	5.6
1	C	92	GLY	5.1
1	A	223	ASN	5.1
1	D	101	LEU	5.0
1	A	246	LEU	5.0
1	C	60	ASP	4.8
1	A	254	THR	4.8
1	B	274	VAL	4.8
1	B	155	THR	4.7
1	B	229	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	28	ASP	4.6
1	D	322	GLU	4.5
1	B	357	ALA	4.4
1	A	78	VAL	4.3
1	D	99	VAL	4.3
1	B	323	GLN	4.2
1	C	91	ALA	4.2
1	C	236	GLN	4.2
1	A	94	PRO	4.1
1	D	59	ALA	4.1
1	C	253	PHE	4.1
1	D	123	ASP	4.1
1	B	226	SER	4.1
1	A	154	ASP	4.0
1	D	295	ASP	4.0
1	D	91	ALA	4.0
1	D	115	LEU	3.9
1	C	215	TRP	3.9
1	A	3	HIS	3.8
1	C	223	ASN	3.8
1	D	50	ILE	3.7
1	C	350	ARG	3.7
1	A	253	PHE	3.7
1	C	357	ALA	3.7
1	A	243	ILE	3.7
1	B	230	GLY	3.7
1	D	58	ASP	3.7
1	B	78	VAL	3.7
1	A	60	ASP	3.7
1	D	221	LEU	3.7
1	D	60	ASP	3.7
1	D	119	GLU	3.6
1	A	81	GLY	3.6
1	D	329	GLY	3.6
1	C	219	ASP	3.6
1	C	222	VAL	3.6
1	D	124	VAL	3.5
1	D	92	GLY	3.5
1	C	42	GLU	3.4
1	C	254	THR	3.4
1	A	220	LYS	3.4
1	B	60	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	36	VAL	3.4
1	D	154	ASP	3.4
1	C	237	ASN	3.4
1	C	243	ILE	3.4
1	C	216	GLY	3.3
1	B	253	PHE	3.3
1	C	116	GLU	3.3
1	D	198	CYS	3.3
1	D	214	THR	3.3
1	D	357	ALA	3.3
1	A	74[A]	GLU	3.2
1	C	95	PRO	3.2
1	D	3	HIS	3.2
1	C	235	ASN	3.2
1	D	224	ARG	3.2
1	D	194	LYS	3.2
1	B	343	GLU	3.1
1	A	322	GLU	3.1
1	B	151	LEU	3.1
1	C	246	LEU	3.1
1	B	85	SER	3.1
1	C	313	ALA	3.1
1	A	323	GLN	3.0
1	D	340	VAL	3.0
1	C	275	THR	3.0
1	A	219	ASP	3.0
1	B	326	ALA	3.0
1	D	215	TRP	3.0
1	C	241	GLU	3.0
1	A	327	LYS	3.0
1	A	321	THR	3.0
1	B	254	THR	3.0
1	D	145	PRO	3.0
1	A	156	ILE	3.0
1	C	303	VAL	2.9
1	D	243	ILE	2.9
1	D	126	TYR	2.9
1	D	356	VAL	2.9
1	B	3[A]	HIS	2.9
1	A	121	SER	2.9
1	D	120	PRO	2.9
1	C	115	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	217	PHE	2.8
1	B	101	LEU	2.8
1	A	343	GLU	2.8
1	A	146	ASP	2.8
1	C	151	LEU	2.8
1	D	220	LYS	2.7
1	C	327	LYS	2.7
1	B	322	GLU	2.7
1	A	202	LEU	2.7
1	C	18	ILE	2.7
1	D	353	VAL	2.7
1	D	34	ILE	2.7
1	A	103	PRO	2.7
1	A	349	LEU	2.7
1	C	94	PRO	2.6
1	A	224	ARG	2.6
1	C	353	VAL	2.5
1	C	44	ASN	2.5
1	D	223	ASN	2.5
1	A	124	VAL	2.5
1	D	65	ARG	2.5
1	D	103	PRO	2.5
1	C	28	ASP	2.5
1	D	325	MET	2.5
1	C	74	GLU	2.5
1	C	349	LEU	2.5
1	D	28	ASP	2.5
1	C	79	GLN	2.5
1	C	27	PRO	2.4
1	C	12	CYS	2.4
1	D	327	LYS	2.4
1	D	147	LEU	2.4
1	D	289	ARG	2.4
1	C	53	LEU	2.4
1	A	182	CYS	2.4
1	B	175	ALA	2.4
1	C	221	LEU	2.4
1	B	353	VAL	2.4
1	D	155	THR	2.4
1	D	74	GLU	2.4
1	A	356	VAL	2.3
1	D	98	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	323	GLN	2.3
1	A	216	GLY	2.3
1	C	54	LEU	2.3
1	B	74	GLU	2.3
1	A	247	PHE	2.3
1	B	118	ALA	2.3
1	B	54	LEU	2.3
1	D	151	LEU	2.3
1	A	7	ILE	2.3
1	D	7	ILE	2.3
1	D	326	ALA	2.3
1	B	221	LEU	2.3
1	D	104	LYS	2.3
1	D	253	PHE	2.3
1	B	225	GLU	2.3
1	A	217	PHE	2.3
1	C	126	TYR	2.2
1	A	92	GLY	2.2
1	C	301	VAL	2.2
1	B	116	GLU	2.2
1	D	96	SER	2.2
1	D	32	ILE	2.2
1	A	155	THR	2.2
1	B	80	TRP	2.2
1	C	49	ASN	2.2
1	A	33	ALA	2.2
1	A	291	GLU	2.2
1	B	235	ASN	2.2
1	B	121	SER	2.2
1	C	36	VAL	2.2
1	D	287	ALA	2.2
1	A	93	PHE	2.2
1	D	93	PHE	2.2
1	A	340	VAL	2.2
1	B	50	ILE	2.2
1	D	63	PHE	2.2
1	A	145	PRO	2.2
1	D	85	SER	2.2
1	B	325	MET	2.1
1	B	195	GLY	2.1
1	C	77	THR	2.1
1	D	216	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	117	GLU	2.1
1	C	322	GLU	2.1
1	A	101	LEU	2.1
1	A	151	LEU	2.1
1	D	25	THR	2.1
1	D	111	ILE	2.1
1	A	105	ARG	2.1
1	A	175	ALA	2.1
1	B	2	VAL	2.1
1	C	218	TYR	2.1
1	C	120	PRO	2.1
1	D	64	PHE	2.1
1	C	43	VAL	2.1
1	D	72	VAL	2.1
1	D	121	SER	2.1
1	C	282	VAL	2.0
1	D	222	VAL	2.0
1	C	93	PHE	2.0
1	C	323	GLN	2.0
1	A	222	VAL	2.0
1	B	222	VAL	2.0
1	D	242	PHE	2.0
1	B	150	LYS	2.0
1	A	120	PRO	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 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(Å^2)	Q<0.9
3	BTB	D	401	14/14	0.85	0.22	57,58,60,61	0
3	BTB	A	401	14/14	0.88	0.32	50,55,57,58	0
2	CA	A	400	1/1	0.91	0.09	63,63,63,63	0
3	BTB	B	401	14/14	0.92	0.17	46,54,60,62	0
2	CA	D	400	1/1	0.94	0.06	60,60,60,60	0
3	BTB	C	401	14/14	0.94	0.23	47,52,57,57	0
2	CA	B	400	1/1	0.94	0.08	62,62,62,62	0
2	CA	C	400	1/1	0.98	0.12	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.