



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:43 PM GMT

PDB ID : 1YGY
Title : Crystal Structure of D-3-Phosphoglycerate dehydrogenase From Mycobacterium tuberculosis
Authors : Dey, S.; Grant, G.A.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2005-01-05
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

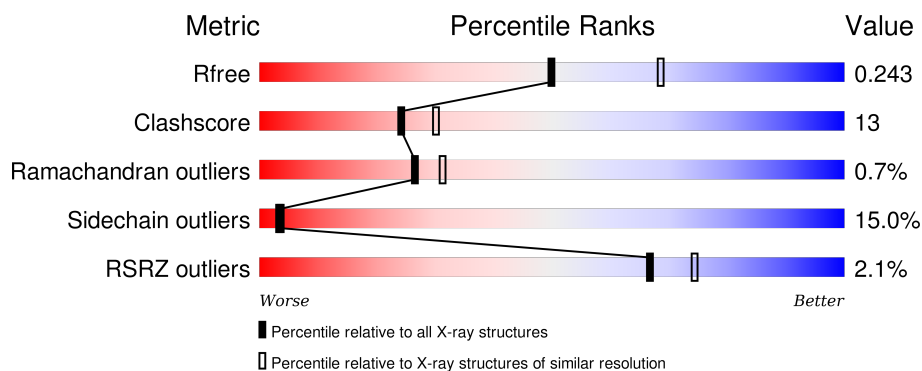
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	529	
1	B	529	

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	TAR	A	600	X	-	-	-
2	TAR	B	1600	X	-	-	-
2	TAR	B	2600	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8017 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.

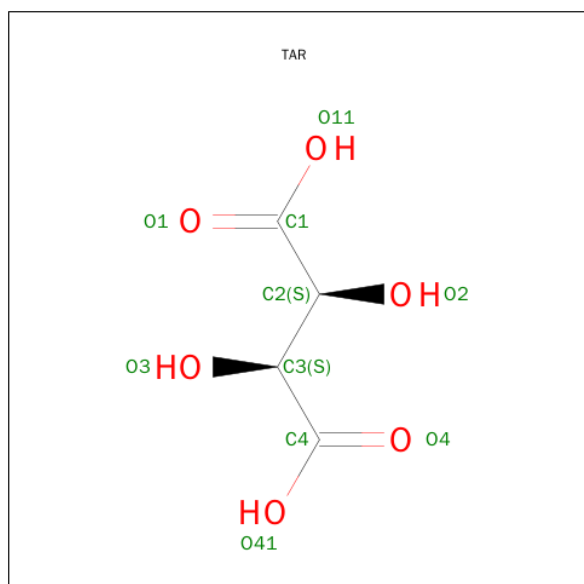
- Molecule 1 is a protein called D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			3836	2416	673	745	2			
1	B	527	Total	C	N	O	S	0	0	0
			3836	2416	673	745	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P0A544
A	2	VAL	-	SEE REMARK 999	UNP P0A544
B	1	MET	-	CLONING ARTIFACT	UNP P0A544
B	2	VAL	-	SEE REMARK 999	UNP P0A544

- Molecule 2 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

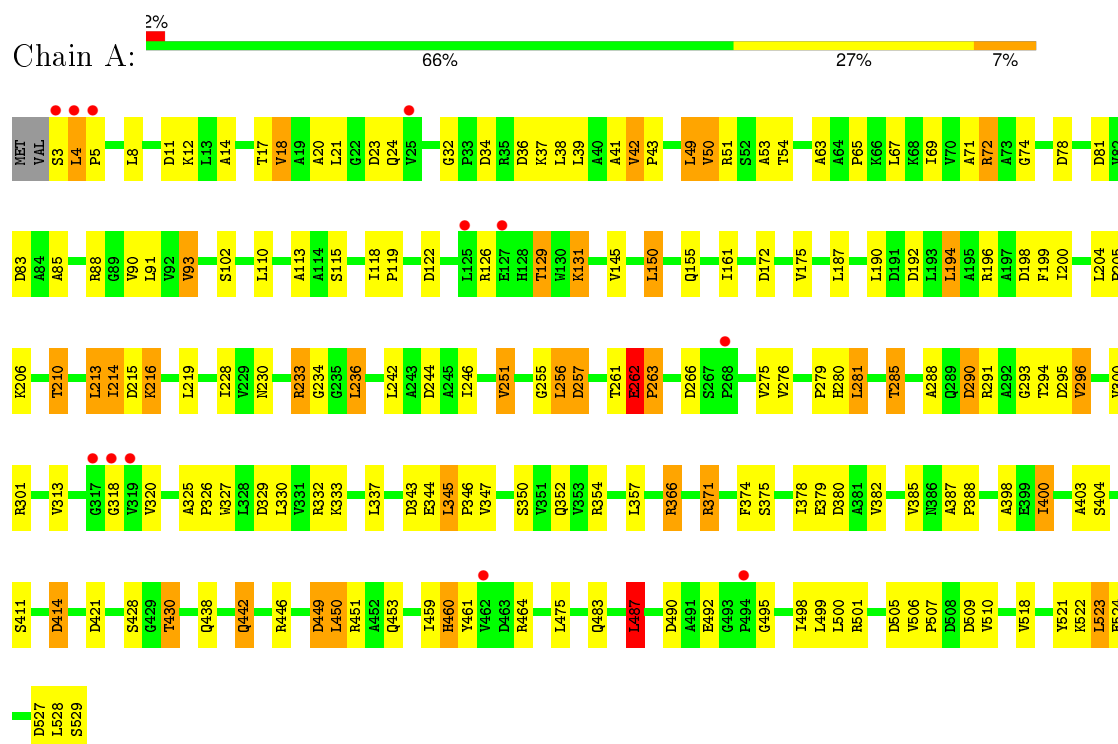
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	151	Total	O	0	0
			151	151		

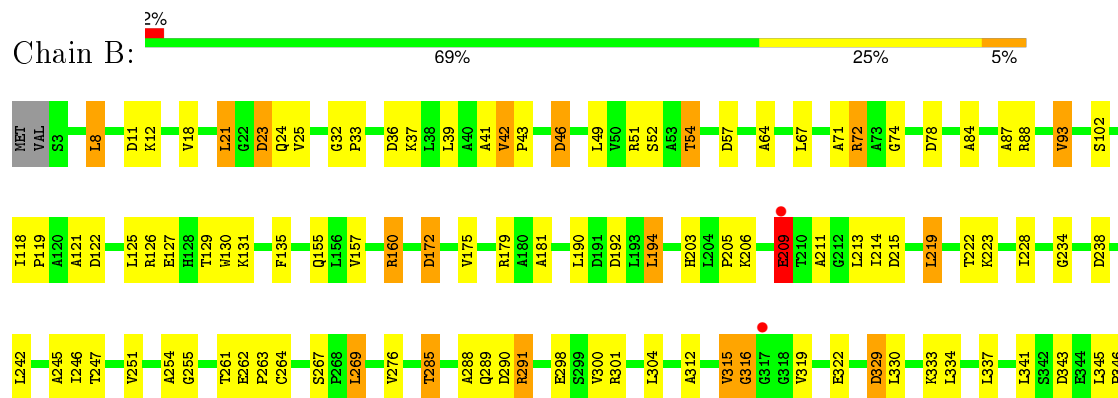
3 Residue-property plots

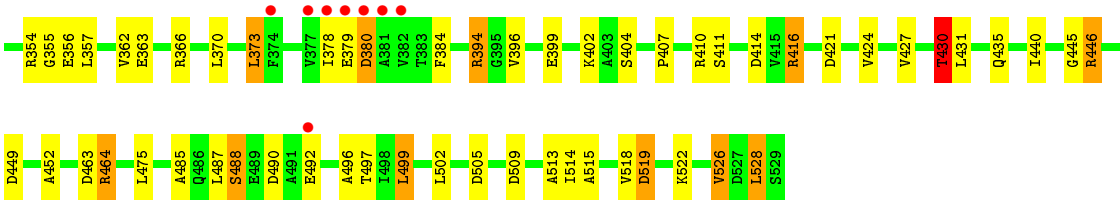
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: D-3-phosphoglycerate dehydrogenase



• Molecule 1: D-3-phosphoglycerate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	165.51Å 165.51Å 218.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.80 – 2.30 48.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.80-2.30) 99.8 (48.52-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.249 0.201 , 0.243	Depositor DCC
R_{free} test set	3932 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 78459 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8017	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TAR

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	0.58	0/3890	0.90	25/5316 (0.5%)
1	B	0.56	0/3890	0.88	20/5316 (0.4%)
All	All	0.57	0/7780	0.89	45/10632 (0.4%)

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	A	0	1
1	B	1	2
All	All	1	3

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	266	ASP	CB-CG-OD2	7.82	125.34	118.30
1	A	215	ASP	CB-CG-OD2	7.74	125.26	118.30
1	A	414	ASP	CB-CG-OD2	7.18	124.77	118.30
1	A	421	ASP	CB-CG-OD2	6.82	124.44	118.30
1	B	46	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	290	ASP	CB-CG-OD2	6.33	123.99	118.30
1	B	57	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	192	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	23	ASP	CB-CG-OD2	6.15	123.84	118.30
1	B	490	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	463	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	36	ASP	CB-CG-OD2	5.96	123.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	198	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	505	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	449	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	122	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	122	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	192	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	83	ASP	CB-CG-OD2	5.58	123.33	118.30
1	B	172	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	343	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	380	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	509	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	449	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	81	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	487	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	238	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	244	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	329	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	34	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	519	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	414	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	295	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	172	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	257	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	78	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	505	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	430	THR	OG1-CB-CG2	5.09	121.71	110.00
1	A	490	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	36	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	290	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	380	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	329	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	527	ASP	CB-CG-OD2	5.02	122.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	430	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	GLU	Peptide
1	B	209	GLU	Peptide
1	B	262	GLU	Peptide

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	3836	0	3921	109	0
1	B	3836	0	3921	95	0
2	A	10	0	4	0	0
2	B	20	0	8	2	0
3	A	164	0	0	4	0
3	B	151	0	0	7	0
All	All	8017	0	7854	202	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 13.

All (202) 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:285:THR:HG22	1:B:288:ALA:H	1.20	1.03
1:A:285:THR:HG22	1:A:288:ALA:H	1.26	1.00
1:B:394:ARG:HH11	1:B:394:ARG:HG2	1.37	0.89
1:A:371:ARG:HH21	1:A:375:SER:CB	1.87	0.88
1:A:459:ILE:HG12	1:A:523:LEU:HD22	1.59	0.85
1:B:285:THR:CG2	1:B:288:ALA:H	1.94	0.80
1:B:362:VAL:HG22	1:B:402:LYS:HD3	1.61	0.80
1:B:315:VAL:HG13	1:B:316:GLY:H	1.45	0.80
1:B:411:SER:O	1:B:430:THR:HG23	1.82	0.80
1:B:315:VAL:HG13	1:B:316:GLY:N	1.99	0.77
1:B:345:LEU:HD12	1:B:346:PRO:HD2	1.66	0.77
1:A:371:ARG:HH21	1:A:375:SER:HB2	1.51	0.75
1:B:362:VAL:CG2	1:B:402:LYS:HD3	2.16	0.75
1:A:499:LEU:C	1:A:499:LEU:HD23	2.07	0.75
1:A:129:THR:HB	1:A:131:LYS:HE2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLU:OE2	1:B:366:ARG:NH1	2.21	0.74
1:B:445:GLY:O	1:B:446:ARG:NH1	2.21	0.73
1:B:118:ILE:HB	1:B:119:PRO:HD3	1.70	0.72
1:A:387:ALA:HB3	1:A:388:PRO:HD3	1.70	0.72
1:A:371:ARG:HH21	1:A:375:SER:HB3	1.54	0.72
1:A:506:VAL:CG1	1:A:510:VAL:HG23	2.20	0.71
1:B:102:SER:OG	1:B:285:THR:HG21	1.90	0.71
1:B:334:LEU:HD22	1:B:427:VAL:HG12	1.73	0.71
1:A:205:PRO:O	1:A:210:THR:HG21	1.89	0.70
1:B:11:ASP:OD1	1:B:54:THR:HG22	1.91	0.70
1:A:506:VAL:HG12	1:A:510:VAL:HG23	1.73	0.69
1:A:50:VAL:HG22	1:A:54:THR:HB	1.75	0.69
1:B:356:GLU:OE1	1:B:410:ARG:HD2	1.95	0.67
1:B:160:ARG:NH1	3:B:2749:HOH:O	2.26	0.66
1:A:506:VAL:HG12	1:A:510:VAL:CG2	2.26	0.66
1:A:18:VAL:HG13	1:A:21:LEU:HD12	1.78	0.65
1:A:42:VAL:N	1:A:43:PRO:CD	2.59	0.65
1:A:483:GLN:OE1	1:A:501:ARG:HD2	1.97	0.64
1:B:206:LYS:HE2	3:B:2738:HOH:O	1.95	0.64
1:B:23:ASP:HB3	1:B:24:GLN:HE21	1.63	0.64
1:A:71:ALA:HB1	1:A:296:VAL:HG22	1.80	0.64
1:B:42:VAL:HG13	1:B:64:ALA:HB2	1.79	0.63
1:A:37:LYS:HE2	3:A:663:HOH:O	1.99	0.62
1:B:526:VAL:HG22	1:B:528:LEU:HD13	1.80	0.62
1:A:506:VAL:CG1	1:A:510:VAL:CG2	2.78	0.62
1:B:354:ARG:HD2	3:B:2648:HOH:O	2.00	0.61
1:A:499:LEU:HD23	1:A:500:LEU:N	2.15	0.61
1:A:460:HIS:HB3	1:A:521:TYR:CZ	2.36	0.61
1:A:313:VAL:HG12	1:A:313:VAL:O	2.01	0.61
1:B:315:VAL:CG1	1:B:316:GLY:N	2.64	0.61
1:B:394:ARG:NH1	1:B:394:ARG:HG2	2.13	0.60
1:A:411:SER:O	1:A:430:THR:CG2	2.50	0.60
1:B:42:VAL:N	1:B:43:PRO:CD	2.64	0.60
1:B:488:SER:HB3	2:B:1600:TAR:H3	1.83	0.60
1:B:394:ARG:CG	1:B:394:ARG:HH11	2.10	0.59
1:A:354:ARG:NH1	1:A:414:ASP:OD1	2.35	0.59
1:B:285:THR:HG22	1:B:288:ALA:N	2.04	0.59
1:A:17:THR:O	1:A:294:THR:HG22	2.04	0.58
1:A:18:VAL:HG13	1:A:18:VAL:O	2.04	0.58
1:A:411:SER:O	1:A:430:THR:HG23	2.04	0.58
1:B:23:ASP:HB3	1:B:24:GLN:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LYS:HE2	1:A:528:LEU:O	2.04	0.57
1:A:200:ILE:HD12	1:A:228:ILE:CD1	2.34	0.57
1:B:119:PRO:HG2	1:B:276:VAL:HG13	1.86	0.56
1:A:507:PRO:O	1:A:510:VAL:HG22	2.05	0.56
1:B:32:GLY:N	1:B:33:PRO:HD2	2.20	0.56
1:A:102:SER:OG	1:A:285:THR:HG21	2.05	0.56
1:A:352:GLN:NE2	1:A:354:ARG:HH11	2.04	0.56
1:A:118:ILE:HB	1:A:119:PRO:HD3	1.88	0.55
1:A:113:ALA:HA	1:A:118:ILE:HG12	1.89	0.55
1:B:446:ARG:HD2	1:B:446:ARG:N	2.22	0.55
1:A:246:ILE:HD13	1:A:251:VAL:HG22	1.90	0.54
1:A:366:ARG:HB2	1:A:400:ILE:HG12	1.89	0.54
1:A:275:VAL:O	1:B:126:ARG:NH2	2.40	0.54
1:A:257:ASP:OD2	1:A:281:LEU:O	2.25	0.53
1:A:50:VAL:CG2	1:A:54:THR:HB	2.38	0.53
1:A:279:PRO:HD2	1:A:281:LEU:HD22	1.89	0.53
1:B:72:ARG:HH11	1:B:74:GLY:HA3	1.74	0.53
1:B:215:ASP:HB2	3:B:2636:HOH:O	2.08	0.53
1:B:430:THR:HG22	1:B:431:LEU:H	1.73	0.53
1:A:371:ARG:NH2	3:A:757:HOH:O	2.25	0.52
1:A:371:ARG:NH2	1:A:375:SER:HB2	2.20	0.52
1:A:41:ALA:C	1:A:43:PRO:HD2	2.30	0.52
1:A:72:ARG:HH11	1:A:74:GLY:HA3	1.74	0.52
1:B:301:ARG:HH11	1:B:301:ARG:HG2	1.75	0.52
1:B:242:LEU:O	1:B:246:ILE:HG12	2.09	0.52
1:B:172:ASP:O	1:B:175:VAL:HG12	2.10	0.52
1:A:498:ILE:HD13	1:A:500:LEU:HD11	1.92	0.51
1:B:346:PRO:O	1:B:396:VAL:HG22	2.10	0.51
1:A:499:LEU:CD2	1:A:499:LEU:C	2.79	0.51
1:B:301:ARG:HG2	1:B:301:ARG:NH1	2.26	0.51
1:B:93:VAL:HG23	1:B:312:ALA:HA	1.93	0.51
1:B:464:ARG:HH11	1:B:464:ARG:HB2	1.76	0.50
1:A:352:GLN:NE2	1:A:354:ARG:NH1	2.59	0.50
1:B:11:ASP:OD1	1:B:54:THR:CG2	2.58	0.50
1:A:262:GLU:HB3	1:A:263:PRO:CD	2.41	0.50
1:B:445:GLY:C	1:B:446:ARG:HD2	2.32	0.50
1:B:255:GLY:HA2	1:B:276:VAL:O	2.11	0.50
1:A:313:VAL:CG1	1:A:313:VAL:O	2.59	0.50
1:B:513:ALA:HA	3:B:2704:HOH:O	2.12	0.49
1:A:71:ALA:HA	1:A:93:VAL:HG12	1.95	0.49
1:B:515:ALA:O	1:B:518:VAL:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ALA:O	1:A:65:PRO:HD3	2.12	0.49
1:B:11:ASP:OD2	1:B:54:THR:HG23	2.12	0.49
1:B:155:GLN:OE1	1:B:179:ARG:HD2	2.12	0.49
1:B:84:ALA:O	1:B:87:ALA:HB3	2.13	0.48
1:B:245:ALA:HB1	1:B:251:VAL:HG23	1.95	0.48
1:B:42:VAL:N	1:B:43:PRO:HD2	2.28	0.48
1:A:233:ARG:HB3	1:A:236:LEU:HD22	1.94	0.48
1:A:49:LEU:CD2	1:A:300:VAL:HG21	2.43	0.48
1:A:498:ILE:CD1	1:A:500:LEU:HD11	2.42	0.48
1:A:206:LYS:HB2	1:A:233:ARG:HG2	1.95	0.48
1:A:313:VAL:HG13	1:A:382:VAL:HA	1.96	0.48
1:B:267:SER:OG	1:B:269:LEU:HB2	2.14	0.48
1:B:41:ALA:C	1:B:43:PRO:HD2	2.35	0.47
1:A:32:GLY:HA3	1:A:54:THR:OG1	2.14	0.47
1:A:464:ARG:NH1	1:A:495:GLY:O	2.44	0.47
1:B:209:GLU:OE2	1:B:211:ALA:HB3	2.15	0.47
1:A:129:THR:HB	1:A:131:LYS:CE	2.42	0.47
1:B:373:LEU:HD22	1:B:373:LEU:O	2.15	0.46
1:A:145:VAL:HG22	1:A:199:PHE:HB2	1.97	0.46
1:A:11:ASP:OD2	1:A:53:ALA:HB3	2.15	0.46
1:A:204:LEU:HD11	1:A:213:LEU:HD12	1.97	0.46
1:B:345:LEU:CD1	1:B:346:PRO:HD2	2.43	0.46
1:B:394:ARG:CG	1:B:394:ARG:NH1	2.70	0.46
1:B:291:ARG:HD3	1:B:291:ARG:HA	1.70	0.46
1:A:332:ARG:HG2	1:A:332:ARG:HH11	1.80	0.46
1:A:150:LEU:HD22	1:A:155:GLN:HG2	1.98	0.46
1:A:233:ARG:CB	1:A:236:LEU:HD22	2.45	0.46
1:A:255:GLY:HA2	1:A:276:VAL:O	2.16	0.46
1:B:121:ALA:HA	1:B:135:PHE:CZ	2.51	0.45
1:B:378:ILE:HG22	1:B:379:GLU:O	2.16	0.45
1:B:190:LEU:O	1:B:194:LEU:HD22	2.15	0.45
1:A:131:LYS:HB2	1:A:131:LYS:HE3	1.54	0.45
1:B:102:SER:HG	1:B:285:THR:HG21	1.80	0.45
1:A:262:GLU:HG2	1:B:130:TRP:CH2	2.51	0.45
1:A:230:ASN:HB3	1:A:256:LEU:HD22	1.98	0.45
1:B:214:ILE:HG22	1:B:219:LEU:HD13	1.97	0.45
1:B:440:ILE:HD11	1:B:452:ALA:HA	1.99	0.45
1:A:190:LEU:HG	1:A:194:LEU:HD22	1.97	0.45
1:A:330:LEU:HD13	1:A:438:GLN:HB3	1.98	0.45
1:A:451:ARG:HB3	1:A:453:GLN:HG2	1.99	0.44
1:A:71:ALA:CB	1:A:93:VAL:HG12	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:O	1:A:214:ILE:HG22	2.16	0.44
1:B:407:PRO:HD2	3:B:2676:HOH:O	2.17	0.44
1:A:161:ILE:HD12	1:A:161:ILE:HA	1.86	0.44
1:B:228:ILE:O	1:B:254:ALA:HA	2.17	0.44
1:A:206:LYS:N	3:A:733:HOH:O	2.25	0.44
1:B:363:GLU:HG2	2:B:2600:TAR:O2	2.17	0.44
1:A:460:HIS:HB3	1:A:521:TYR:CE1	2.53	0.44
1:A:246:ILE:CD1	1:A:251:VAL:HG22	2.48	0.43
1:B:51:ARG:HD3	1:B:289:GLN:OE1	2.19	0.43
1:B:514:ILE:O	1:B:518:VAL:HG22	2.18	0.43
1:B:21:LEU:HA	1:B:21:LEU:HD12	1.77	0.43
1:A:487:LEU:HB3	1:A:498:ILE:HG13	2.00	0.43
1:A:131:LYS:HE3	1:A:131:LYS:N	2.34	0.43
1:B:329:ASP:O	1:B:333:LYS:HG3	2.19	0.43
1:A:42:VAL:N	1:A:43:PRO:HD3	2.33	0.43
1:A:366:ARG:HG3	1:A:398:ALA:HB1	2.01	0.43
1:B:181:ALA:HB3	3:B:2739:HOH:O	2.18	0.43
1:A:4:LEU:HA	1:A:5:PRO:HD3	1.87	0.43
1:A:261:THR:HG23	1:A:261:THR:O	2.19	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.92	0.43
1:B:157:VAL:HG21	1:B:203:HIS:CE1	2.54	0.43
1:A:216:LYS:HE2	1:A:216:LYS:HB2	1.46	0.42
1:A:352:GLN:HE21	1:A:354:ARG:NH1	2.18	0.42
1:A:528:LEU:HD23	1:A:528:LEU:HA	1.65	0.42
1:B:300:VAL:O	1:B:304:LEU:HG	2.20	0.42
1:A:403:ALA:HA	3:A:615:HOH:O	2.19	0.42
1:B:8:LEU:HD23	1:B:8:LEU:HA	1.83	0.42
1:A:318:GLY:O	1:A:320:VAL:N	2.52	0.42
1:A:442:GLN:HA	1:A:446:ARG:O	2.20	0.42
1:A:18:VAL:CG1	1:A:18:VAL:O	2.68	0.42
1:A:327:TRP:CE2	1:A:357:LEU:HD22	2.55	0.42
1:A:460:HIS:HB2	1:A:522:LYS:HB3	2.01	0.41
1:A:461:TYR:CD2	1:A:518:VAL:HB	2.55	0.41
1:B:485:ALA:HA	1:B:499:LEU:O	2.19	0.41
1:A:290:ASP:O	1:A:294:THR:HG23	2.20	0.41
1:B:49:LEU:HD21	1:B:300:VAL:HG21	2.01	0.41
1:B:127:GLU:O	1:B:129:THR:HG23	2.20	0.41
1:A:17:THR:CG2	1:A:293:GLY:HA3	2.50	0.41
1:A:257:ASP:O	1:A:280:HIS:HA	2.21	0.41
1:B:435:GLN:OE1	1:B:435:GLN:HA	2.20	0.41
1:A:449:ASP:O	1:A:450:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ALA:O	1:A:17:THR:HB	2.21	0.41
1:B:205:PRO:HG3	1:B:211:ALA:HB2	2.02	0.41
1:A:20:ALA:O	1:A:301:ARG:HD3	2.20	0.41
1:A:366:ARG:HG3	1:A:398:ALA:CB	2.51	0.41
1:B:51:ARG:O	1:B:72:ARG:NE	2.53	0.41
1:B:194:LEU:O	1:B:222:THR:HA	2.20	0.41
1:A:49:LEU:HD22	1:A:300:VAL:HG21	2.02	0.41
1:A:150:LEU:HB3	1:A:175:VAL:HG21	2.02	0.41
1:B:440:ILE:CD1	1:B:452:ALA:HA	2.51	0.41
1:B:487:LEU:HD11	1:B:496:ALA:HB1	2.01	0.41
1:A:374:PHE:O	1:A:378:ILE:HG13	2.21	0.41
1:A:345:LEU:HD22	1:A:346:PRO:HD2	2.03	0.41
1:B:373:LEU:HD23	1:B:373:LEU:HA	1.81	0.41
1:B:416:ARG:NH1	1:B:424:VAL:HG11	2.36	0.41
1:B:261:THR:O	1:B:264:CYS:HB2	2.20	0.41
1:B:49:LEU:HD22	1:B:71:ALA:HB3	2.03	0.40
1:B:355:GLY:HA2	1:B:404:SER:O	2.21	0.40
1:A:85:ALA:HB1	1:A:90:VAL:HB	2.03	0.40
1:A:325:ALA:HB3	1:A:326:PRO:HD3	2.03	0.40
1:B:285:THR:HG22	1:B:285:THR:O	2.21	0.40
1:A:118:ILE:HB	1:A:119:PRO:CD	2.49	0.40
1:B:298:GLU:OE2	1:B:298:GLU:HA	2.22	0.40
1:B:528:LEU:HA	1:B:528:LEU:HD12	1.80	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	525/529 (99%)	490 (93%)	32 (6%)	3 (1%)	30	36
1	B	525/529 (99%)	490 (93%)	31 (6%)	4 (1%)	24	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1050/1058 (99%)	980 (93%)	63 (6%)	7 (1%)	26	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	PRO
1	B	263	PRO
1	B	316	GLY
1	A	262	GLU
1	B	234	GLY
1	B	380	ASP
1	A	234	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	397/399 (100%)	333 (84%)	64 (16%)	3	3
1	B	397/399 (100%)	342 (86%)	55 (14%)	4	4
All	All	794/798 (100%)	675 (85%)	119 (15%)	3	3

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	LEU
1	A	8	LEU
1	A	12	LYS
1	A	18	VAL
1	A	24	GLN
1	A	38	LEU
1	A	39	LEU
1	A	42	VAL
1	A	49	LEU
1	A	50	VAL

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Mol	Chain	Res	Type
1	A	51	ARG
1	A	67	LEU
1	A	69	ILE
1	A	72	ARG
1	A	78	ASP
1	A	88	ARG
1	A	91	LEU
1	A	93	VAL
1	A	110	LEU
1	A	115	SER
1	A	126	ARG
1	A	129	THR
1	A	131	LYS
1	A	150	LEU
1	A	194	LEU
1	A	196	ARG
1	A	210	THR
1	A	213	LEU
1	A	214	ILE
1	A	216	LYS
1	A	219	LEU
1	A	233	ARG
1	A	236	LEU
1	A	242	LEU
1	A	251	VAL
1	A	256	LEU
1	A	281	LEU
1	A	285	THR
1	A	291	ARG
1	A	296	VAL
1	A	337	LEU
1	A	344	GLU
1	A	345	LEU
1	A	347	VAL
1	A	350	SER
1	A	366	ARG
1	A	371	ARG
1	A	379	GLU
1	A	385	VAL
1	A	400	ILE
1	A	404	SER
1	A	428	SER

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Mol	Chain	Res	Type
1	A	430	THR
1	A	442	GLN
1	A	450	LEU
1	A	460	HIS
1	A	475	LEU
1	A	487	LEU
1	A	492	GLU
1	A	509	ASP
1	A	523	LEU
1	A	524	GLU
1	A	529	SER
1	B	8	LEU
1	B	12	LYS
1	B	18	VAL
1	B	21	LEU
1	B	23	ASP
1	B	25	VAL
1	B	37	LYS
1	B	39	LEU
1	B	42	VAL
1	B	46	ASP
1	B	52	SER
1	B	54	THR
1	B	67	LEU
1	B	72	ARG
1	B	88	ARG
1	B	93	VAL
1	B	125	LEU
1	B	131	LYS
1	B	160	ARG
1	B	194	LEU
1	B	209	GLU
1	B	213	LEU
1	B	219	LEU
1	B	223	LYS
1	B	247	THR
1	B	269	LEU
1	B	285	THR
1	B	291	ARG
1	B	315	VAL
1	B	319	VAL
1	B	322	GLU

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Mol	Chain	Res	Type
1	B	330	LEU
1	B	337	LEU
1	B	341	LEU
1	B	343	ASP
1	B	357	LEU
1	B	370	LEU
1	B	373	LEU
1	B	384	PHE
1	B	394	ARG
1	B	399	GLU
1	B	416	ARG
1	B	430	THR
1	B	446	ARG
1	B	464	ARG
1	B	475	LEU
1	B	488	SER
1	B	492	GLU
1	B	497	THR
1	B	499	LEU
1	B	502	LEU
1	B	519	ASP
1	B	522	LYS
1	B	526	VAL
1	B	528	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	435	GLN
1	B	24	GLN
1	B	321	ASN
1	B	408	ASN
1	B	442	GLN
1	B	504	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	TAR	A	600	-	3,9,9	0.31	0	6,12,12	0.79	0
2	TAR	B	1600	-	3,9,9	0.19	0	6,12,12	1.31	2 (33%)
2	TAR	B	2600	-	3,9,9	0.15	0	6,12,12	1.55	2 (33%)

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	TAR	A	600	-	2/2/4/4	0/4/12/12	0/0/0/0
2	TAR	B	1600	-	2/2/4/4	0/4/12/12	0/0/0/0
2	TAR	B	2600	-	2/2/4/4	0/4/12/12	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2600	TAR	C1-C2-C3	-2.68	107.85	113.35
2	B	2600	TAR	C4-C3-C2	-2.68	107.86	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1600	TAR	C4-C3-C2	-2.35	108.54	113.35
2	B	1600	TAR	C1-C2-C3	-2.02	109.20	113.35

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	600	TAR	C2
2	A	600	TAR	C3
2	B	2600	TAR	C2
2	B	2600	TAR	C3
2	B	1600	TAR	C2
2	B	1600	TAR	C3

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1600	TAR	1	0
2	B	2600	TAR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	527/529 (99%)	-0.27	12 (2%) 64 72	11, 32, 56, 79	0
1	B	527/529 (99%)	-0.34	10 (1%) 70 76	13, 33, 63, 100	0
All	All	1054/1058 (99%)	-0.30	22 (2%) 67 74	11, 32, 60, 100	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	VAL	5.7
1	B	317	GLY	5.5
1	B	380	ASP	4.8
1	A	4	LEU	4.7
1	B	492	GLU	4.5
1	B	379	GLU	4.1
1	B	381	ALA	3.8
1	A	318	GLY	3.7
1	B	382	VAL	3.5
1	A	462	VAL	3.4
1	B	377	VAL	3.4
1	A	125	LEU	3.4
1	B	209	GLU	3.2
1	B	374	PHE	3.0
1	A	25	VAL	2.9
1	A	3	SER	2.5
1	B	378	ILE	2.4
1	A	317	GLY	2.2
1	A	127	GLU	2.2
1	A	5	PRO	2.2
1	A	494	PRO	2.1
1	A	268	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	TAR	A	600	10/10	0.95	0.11	0.30	66,72,79,83	0
2	TAR	B	1600	10/10	0.96	0.10	-0.25	59,70,75,77	0
2	TAR	B	2600	10/10	0.94	0.15	-	54,63,67,69	10

6.5 Other polymers [i](#)

There are no such residues in this entry.