



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:02 PM UTC

PDB ID : 3DDN / pdb_00003ddn
Title : Crystal structure of hydroxypyruvic acid phosphate bound D-3-phosphoglycerate dehydrogenase in mycobacterium tuberculosis
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2008-06-05
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

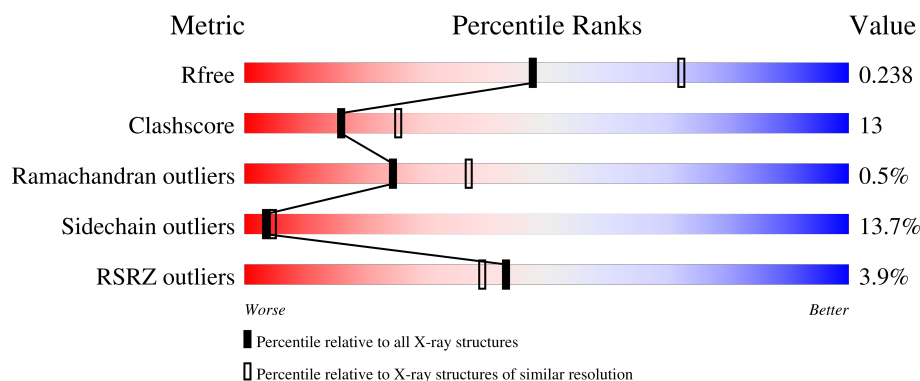
1 Overall quality at a glance

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	528	2% 73% 21% 5%
1	B	528	5% 74% 21% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7889 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.

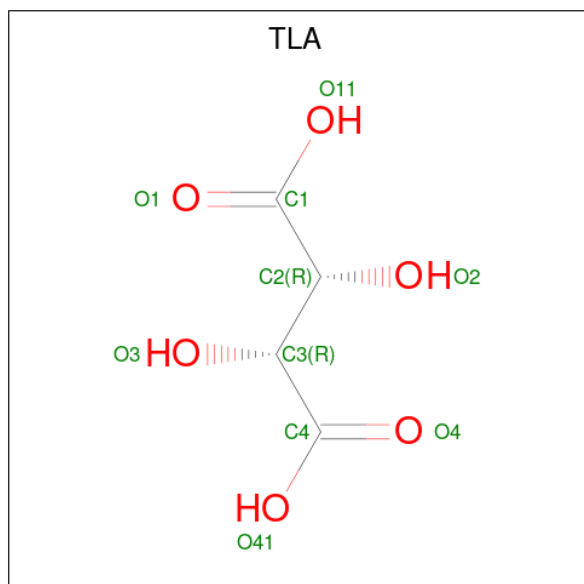
- Molecule 1 is a protein called D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	4	0
			3860	2432	677	749	2			
1	B	525	Total	C	N	O	S	0	0	0
			3823	2409	671	741	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	-	expression tag	UNP P0A544
B	2	VAL	-	expression tag	UNP P0A544

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



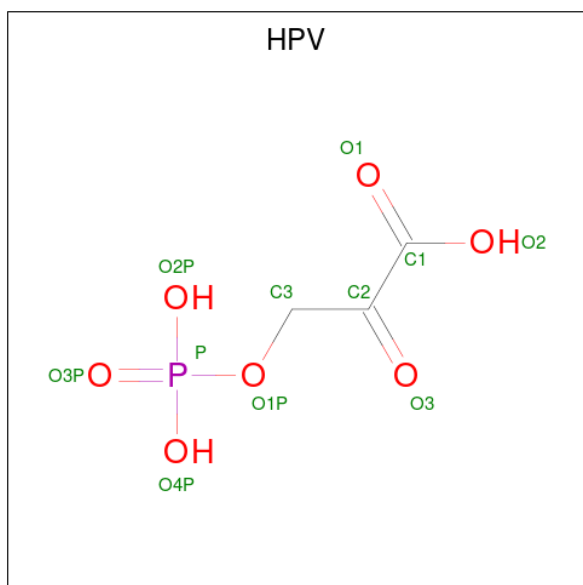
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 2-oxo-3-(phosphonooxy)propanoic acid (CCD ID: HPV) (formula: $C_3H_5O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			11	3	7	1		

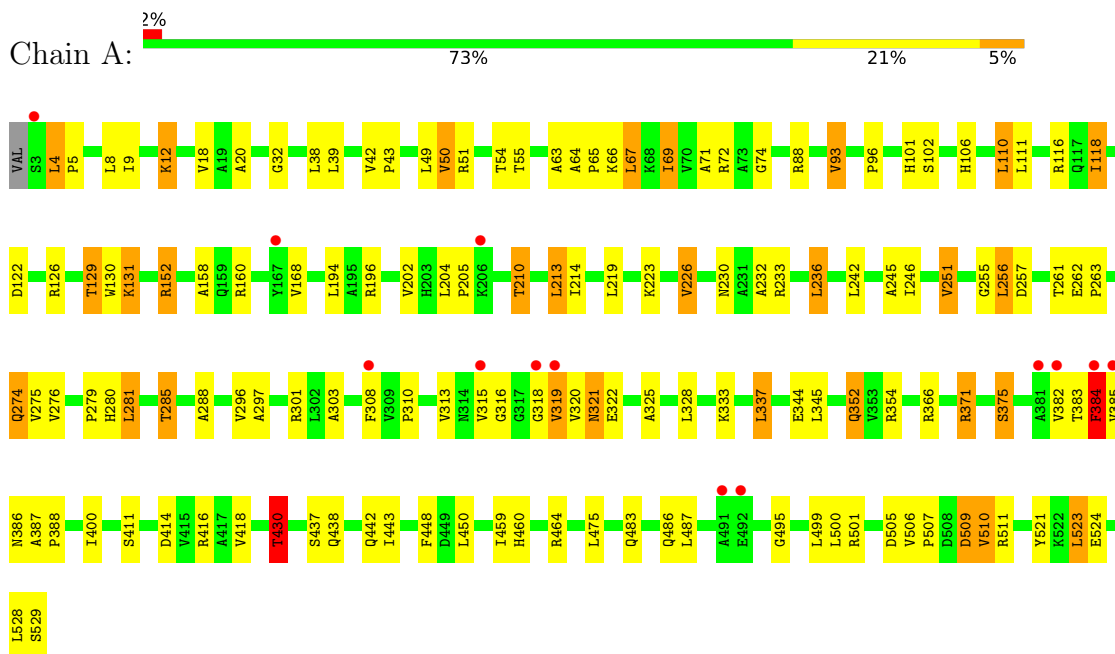
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	72	Total	O	0	0
			72	72		

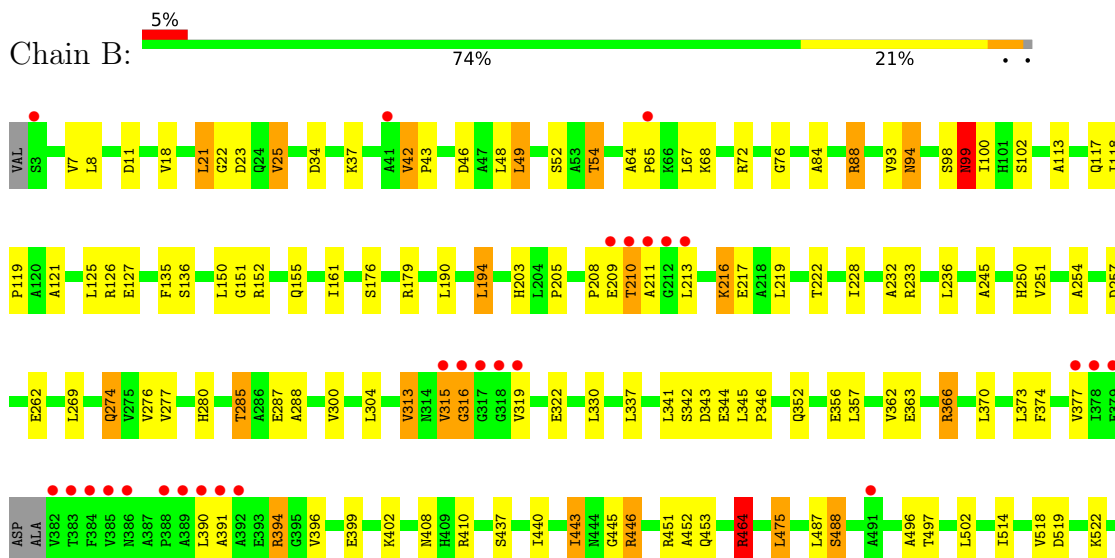
3 Residue-property plots [i](#)

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: 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	165.60Å 165.60Å 218.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.79 – 2.40 48.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.79-2.40) 99.9 (48.79-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.244 0.199 , 0.238	Depositor DCC
R_{free} test set	3485 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7889	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: HPV, TLA

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	0.73	1/3932 (0.0%)	0.98	2/5372 (0.0%)
1	B	0.69	0/3876	1.00	13/5295 (0.2%)
All	All	0.71	1/7808 (0.0%)	0.99	15/10667 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	ALA	CA-CB	5.09	1.58	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	SER	CA-C-N	9.13	132.52	120.28
1	B	98	SER	C-N-CA	9.13	132.52	120.28
1	B	464	ARG	CA-C-N	-7.39	112.17	119.78
1	B	464	ARG	C-N-CA	-7.39	112.17	119.78
1	A	430	THR	CB-CA-C	-6.50	97.43	110.30
1	B	99	ASN	N-CA-C	6.31	118.16	111.28
1	B	443	ILE	CB-CA-C	-6.20	103.35	110.73
1	A	384	PHE	N-CA-C	-6.04	100.45	110.17
1	B	100	ILE	N-CA-C	5.58	115.78	110.42
1	B	99	ASN	CB-CA-C	-5.42	101.79	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ASP	N-CA-C	5.41	117.17	111.28
1	B	518	VAL	N-CA-C	5.39	117.59	111.88
1	B	22	GLY	CA-C-N	5.14	127.16	120.28
1	B	22	GLY	C-N-CA	5.14	127.16	120.28
1	B	313	VAL	N-CA-CB	-5.10	106.60	112.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	99	ASN	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	3860	0	3941	107	0
1	B	3823	0	3911	102	0
2	A	10	0	4	0	0
2	B	20	0	8	1	0
3	B	11	0	2	3	0
4	A	93	0	0	2	0
4	B	72	0	0	0	0
All	All	7889	0	7866	206	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 (206) 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:274:GLN:H	1:B:274:GLN:NE2	1.40	1.17
1:B:274:GLN:HE21	1:B:274:GLN:N	1.44	1.15
1:A:285:THR:HG22	1:A:288:ALA:H	1.20	1.06
1:B:285:THR:HG22	1:B:288:ALA:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352[A]:GLN:HE22	1:A:416:ARG:HD3	1.36	0.89
1:A:205:PRO:O	1:A:210:THR:HG21	1.73	0.88
1:B:72:ARG:HH12	3:B:600:HPV:H3	1.41	0.86
1:A:352[A]:GLN:HE22	1:A:416:ARG:CD	1.88	0.85
1:B:11:ASP:OD1	1:B:54:THR:HG22	1.79	0.83
1:A:50:VAL:HG22	1:A:54:THR:HB	1.61	0.82
1:A:129:THR:HB	1:A:131:LYS:NZ	1.94	0.82
1:A:411:SER:O	1:A:430:THR:CG2	2.30	0.79
1:A:411:SER:O	1:A:430:THR:HG23	1.82	0.78
1:B:216:LYS:HD2	1:B:217:GLU:N	1.98	0.77
1:A:230:ASN:ND2	1:A:232:ALA:H	1.81	0.77
1:A:274:GLN:H	1:A:274:GLN:NE2	1.82	0.76
1:B:285:THR:CG2	1:B:288:ALA:H	1.99	0.75
1:A:352[A]:GLN:NE2	1:A:416:ARG:HD3	2.00	0.75
1:B:155:GLN:HE22	1:B:179:ARG:HH11	1.34	0.74
1:B:345:LEU:HD12	1:B:346:PRO:HD2	1.69	0.73
1:B:102:SER:OG	1:B:285:THR:HG21	1.88	0.73
1:A:129:THR:HB	1:A:131:LYS:CE	2.19	0.72
1:B:42:VAL:HG13	1:B:64:ALA:HB2	1.71	0.72
1:A:129:THR:HB	1:A:131:LYS:HE2	1.73	0.71
1:B:11:ASP:OD2	1:B:54:THR:HG23	1.92	0.70
1:B:210:THR:HG22	1:B:210:THR:O	1.91	0.70
1:B:362:VAL:CG2	1:B:402:LYS:HD3	2.23	0.69
1:A:499:LEU:HD23	1:A:499:LEU:C	2.18	0.69
1:B:117:GLN:HE22	1:B:136:SER:H	1.39	0.68
1:A:122:ASP:CG	1:A:126:ARG:HH21	2.02	0.68
1:A:459:ILE:HG12	1:A:523:LEU:HD22	1.77	0.67
1:B:488:SER:HB3	2:B:530:TLA:H3	1.75	0.67
1:A:460:HIS:HB3	1:A:521:TYR:CZ	2.30	0.66
1:A:210:THR:CG2	1:A:236:LEU:HD11	2.25	0.66
1:B:440:ILE:HD11	1:B:452:ALA:HA	1.77	0.66
1:B:362:VAL:HG22	1:B:402:LYS:HD3	1.76	0.66
1:B:440:ILE:CD1	1:B:452:ALA:HA	2.26	0.65
1:B:42:VAL:N	1:B:43:PRO:HD2	2.12	0.65
1:B:52:SER:HB3	1:B:72:ARG:NH2	2.12	0.65
1:B:205:PRO:HG3	1:B:211:ALA:HB2	1.80	0.63
1:A:50:VAL:CG2	1:A:54:THR:HB	2.27	0.63
1:A:274:GLN:H	1:A:274:GLN:HE21	1.45	0.62
1:A:279:PRO:HD2	1:A:281:LEU:HD22	1.81	0.61
1:A:318:GLY:O	1:A:320:VAL:N	2.35	0.60
1:A:316:GLY:N	1:A:319:VAL:HG21	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LYS:NZ	1:A:438:GLN:HE22	2.00	0.59
1:B:11:ASP:CG	1:B:54:THR:CG2	2.75	0.59
1:A:448:PHE:CG	1:A:486:GLN:HG3	2.38	0.59
1:A:223:LYS:O	1:A:226:VAL:HG22	2.03	0.58
1:A:483:GLN:OE1	1:A:501:ARG:HD2	2.03	0.58
1:B:345:LEU:CD1	1:B:346:PRO:HD2	2.34	0.58
1:A:262:GLU:OE2	1:A:280:HIS:ND1	2.26	0.57
1:A:111:LEU:C	1:A:111:LEU:HD23	2.29	0.57
1:B:356:GLU:OE1	1:B:410:ARG:HD2	2.04	0.57
1:B:11:ASP:OD1	1:B:54:THR:CG2	2.50	0.57
1:B:222:THR:O	1:B:250:HIS:NE2	2.35	0.57
1:B:464:ARG:HH22	1:B:519:ASP:HB2	1.70	0.57
1:A:262:GLU:HA	1:A:263:PRO:C	2.30	0.56
1:A:12:LYS:HD3	1:A:12:LYS:N	2.20	0.56
1:A:354:ARG:NH1	1:A:414:ASP:OD1	2.38	0.56
1:A:387:ALA:HB3	1:A:388:PRO:HD3	1.87	0.56
1:B:72:ARG:NH1	3:B:600:HPV:H3	2.14	0.56
1:B:209:GLU:C	1:B:211:ALA:H	2.14	0.56
1:A:245:ALA:HB1	1:A:251:VAL:HG13	1.86	0.56
1:B:72:ARG:HH12	3:B:600:HPV:C3	2.17	0.56
1:B:445:GLY:O	1:B:446:ARG:NH2	2.38	0.56
1:B:245:ALA:HB1	1:B:251:VAL:HG23	1.88	0.56
1:B:190:LEU:O	1:B:194:LEU:HD22	2.05	0.56
1:B:451:ARG:HB3	1:B:453:GLN:HG2	1.88	0.55
1:A:230:ASN:HB3	1:A:256:LEU:HD22	1.89	0.55
1:B:152:ARG:HH11	1:B:155:GLN:NE2	2.04	0.55
1:B:42:VAL:HG12	1:B:43:PRO:HD3	1.90	0.54
1:A:101:HIS:HE1	4:A:754:HOH:O	1.90	0.54
1:B:366:ARG:HH11	1:B:366:ARG:HB3	1.73	0.54
1:A:275:VAL:O	1:B:126:ARG:NH2	2.40	0.54
1:A:204:LEU:HD11	1:A:213:LEU:HD12	1.89	0.53
1:A:313:VAL:HG13	1:A:382:VAL:HA	1.90	0.53
1:B:118:ILE:HB	1:B:119:PRO:HD3	1.90	0.53
1:B:94:ASN:H	1:B:94:ASN:HD22	1.57	0.53
1:A:226:VAL:HG23	1:A:251:VAL:HB	1.89	0.53
1:B:152:ARG:HH11	1:B:155:GLN:HE21	1.57	0.53
1:B:208:PRO:HB3	1:B:209:GLU:OE1	2.09	0.53
1:A:32:GLY:HA3	1:A:54:THR:OG1	2.10	0.52
1:B:52:SER:HB3	1:B:72:ARG:HH21	1.74	0.52
1:A:69:ILE:HD13	1:A:303:ALA:CB	2.39	0.52
1:A:352[B]:GLN:HG2	1:A:354:ARG:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:HD23	1:A:500:LEU:N	2.25	0.52
1:A:464:ARG:NH2	1:A:495:GLY:O	2.41	0.52
1:B:155:GLN:HE22	1:B:179:ARG:NH1	2.06	0.51
1:A:42:VAL:N	1:A:43:PRO:CD	2.73	0.51
1:B:34:ASP:OD2	1:B:37:LYS:HD2	2.10	0.51
1:A:321:ASN:OD1	1:A:322:GLU:N	2.43	0.51
1:A:72:ARG:HH11	1:A:74:GLY:HA3	1.75	0.51
1:B:42:VAL:N	1:B:43:PRO:CD	2.73	0.51
1:A:382:VAL:HG12	1:A:384:PHE:O	2.10	0.51
1:B:117:GLN:NE2	1:B:136:SER:H	2.08	0.51
1:A:116:ARG:HB2	1:A:118:ILE:CD1	2.41	0.50
1:B:440:ILE:CD1	1:B:452:ALA:CA	2.89	0.50
1:A:230:ASN:HD22	1:A:232:ALA:H	1.57	0.50
1:B:209:GLU:C	1:B:211:ALA:N	2.70	0.50
1:B:46:ASP:OD1	1:B:68:LYS:NZ	2.45	0.49
1:B:487:LEU:HD11	1:B:496:ALA:HB1	1.95	0.49
1:A:63:ALA:O	1:A:65:PRO:HD3	2.13	0.49
1:B:209:GLU:O	1:B:211:ALA:N	2.45	0.49
1:A:352[A]:GLN:CD	1:A:416:ARG:HD3	2.38	0.48
1:A:442:GLN:HG2	1:A:443:ILE:N	2.28	0.48
1:B:210:THR:O	1:B:210:THR:CG2	2.61	0.48
1:B:366:ARG:HH11	1:B:366:ARG:CG	2.26	0.48
1:B:216:LYS:HD2	1:B:217:GLU:H	1.77	0.48
1:B:119:PRO:HG2	1:B:276:VAL:HG13	1.95	0.48
1:A:232:ALA:O	1:A:233:ARG:HD2	2.14	0.48
1:B:440:ILE:HD11	1:B:452:ALA:CA	2.44	0.48
1:A:102:SER:OG	1:A:285:THR:HG21	2.14	0.47
1:A:257:ASP:O	1:A:280:HIS:HA	2.12	0.47
1:A:354:ARG:CZ	1:A:414:ASP:OD1	2.62	0.47
1:A:255:GLY:O	1:A:256:LEU:HD23	2.13	0.47
1:B:11:ASP:OD2	1:B:54:THR:CG2	2.62	0.47
1:B:440:ILE:HD12	1:B:440:ILE:N	2.29	0.47
1:A:116:ARG:HB2	1:A:118:ILE:HD11	1.96	0.47
1:A:69:ILE:HD13	1:A:303:ALA:HB3	1.95	0.47
1:A:333:LYS:HZ1	1:A:438:GLN:HE22	1.62	0.46
1:B:72:ARG:HD3	1:B:76:GLY:O	2.14	0.46
1:A:316:GLY:H	1:A:319:VAL:HG21	1.80	0.46
1:B:440:ILE:HD11	1:B:452:ALA:CB	2.46	0.46
1:A:71:ALA:HA	1:A:93:VAL:HG12	1.96	0.46
1:A:131:LYS:HE3	1:A:131:LYS:HB2	1.68	0.46
1:A:509:ASP:OD1	1:A:509:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HB2	1:A:400:ILE:HG12	1.97	0.46
1:A:333:LYS:NZ	1:A:438:GLN:NE2	2.64	0.46
1:A:106:HIS:CD2	1:A:110:LEU:HD22	2.51	0.46
1:B:48:LEU:C	1:B:49:LEU:HD23	2.40	0.46
1:B:72:ARG:CD	1:B:76:GLY:O	2.64	0.46
1:A:386:ASN:OD1	1:A:388:PRO:HD2	2.16	0.45
1:A:210:THR:HG23	1:A:236:LEU:HD11	1.98	0.45
1:A:130:TRP:CH2	1:B:262:GLU:HG2	2.51	0.45
1:A:255:GLY:HA2	1:A:276:VAL:O	2.15	0.45
1:A:507:PRO:O	1:A:510:VAL:HG13	2.16	0.45
1:B:203:HIS:HA	1:B:232:ALA:HB2	1.99	0.45
1:B:464:ARG:NH2	1:B:519:ASP:OD2	2.49	0.45
1:B:257:ASP:O	1:B:280:HIS:HA	2.17	0.45
1:A:285:THR:HG22	1:A:288:ALA:N	2.05	0.44
1:A:352[A]:GLN:HE22	1:A:416:ARG:HD2	1.77	0.44
1:B:88:ARG:H	1:B:88:ARG:HG2	1.61	0.44
1:B:315:VAL:HG13	1:B:316:GLY:N	2.32	0.44
1:A:246:ILE:HG23	1:A:274:GLN:CG	2.48	0.44
1:A:42:VAL:HG22	1:A:64:ALA:HB2	2.00	0.44
1:B:390:LEU:O	1:B:394:ARG:HD2	2.18	0.44
1:B:475:LEU:HD13	1:B:514:ILE:HD11	1.99	0.44
1:A:4:LEU:HA	1:A:5:PRO:HD3	1.84	0.44
1:A:318:GLY:O	1:A:319:VAL:C	2.60	0.44
1:A:507:PRO:O	1:A:511:ARG:HG3	2.17	0.44
1:B:208:PRO:HA	1:B:209:GLU:HA	1.41	0.44
1:B:464:ARG:NH2	1:B:519:ASP:HB2	2.33	0.44
1:A:18:VAL:HG23	1:A:297:ALA:HB2	2.00	0.44
1:B:49:LEU:HD23	1:B:49:LEU:N	2.32	0.44
1:B:203:HIS:HA	1:B:232:ALA:CB	2.48	0.44
1:A:129:THR:CB	1:A:131:LYS:NZ	2.73	0.43
1:B:304:LEU:HD23	1:B:304:LEU:HA	1.87	0.43
1:A:160:ARG:NH2	1:A:160:ARG:HG3	2.34	0.43
1:B:155:GLN:NE2	1:B:179:ARG:HH11	2.08	0.43
1:A:505:ASP:OD2	1:A:506:VAL:N	2.49	0.43
1:B:440:ILE:CD1	1:B:452:ALA:HB2	2.48	0.43
1:A:129:THR:HB	1:A:131:LYS:HZ3	1.78	0.43
1:A:152:ARG:HA	1:A:152:ARG:HD2	1.74	0.43
1:A:204:LEU:CD1	1:A:213:LEU:HD12	2.48	0.43
1:B:362:VAL:O	1:B:363:GLU:C	2.61	0.43
1:A:118:ILE:N	1:A:118:ILE:HD13	2.34	0.42
1:B:176:SER:HB3	1:B:179:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:PHE:O	1:A:310:PRO:HD3	2.20	0.42
1:B:64:ALA:HA	1:B:65:PRO:HD2	1.89	0.42
1:A:210:THR:HG23	1:A:236:LEU:CD1	2.49	0.42
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.77	0.42
1:A:158:ALA:HB1	1:A:168:VAL:HG11	2.02	0.42
1:A:129:THR:HB	1:A:131:LYS:HZ1	1.80	0.42
1:B:150:LEU:C	1:B:151:GLY:O	2.59	0.42
1:A:210:THR:CG2	1:A:236:LEU:CD1	2.95	0.42
1:B:366:ARG:HH11	1:B:366:ARG:CB	2.32	0.42
1:B:216:LYS:HD2	1:B:216:LYS:C	2.45	0.42
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.91	0.41
1:B:49:LEU:HD21	1:B:300:VAL:HG21	2.01	0.41
1:B:274:GLN:H	1:B:274:GLN:HE21	0.61	0.41
1:B:440:ILE:HD12	1:B:452:ALA:HB2	2.01	0.41
1:A:96:PRO:HD2	4:A:703:HOH:O	2.19	0.41
1:A:315:VAL:HG13	1:A:319:VAL:CG2	2.50	0.41
1:B:7:VAL:CG2	1:B:25:VAL:HG11	2.50	0.41
1:B:11:ASP:CG	1:B:54:THR:HG22	2.41	0.41
1:B:113:ALA:HA	1:B:118:ILE:HG12	2.01	0.41
1:B:228:ILE:O	1:B:254:ALA:HA	2.20	0.41
1:A:20:ALA:O	1:A:301:ARG:HD3	2.21	0.41
1:A:122:ASP:OD2	1:A:126:ARG:NH2	2.50	0.41
1:B:21:LEU:HD12	1:B:21:LEU:HA	1.94	0.41
1:B:121:ALA:HA	1:B:135:PHE:CZ	2.55	0.41
1:A:337:LEU:HD13	1:A:528:LEU:HD21	2.01	0.41
1:A:313:VAL:O	1:A:313:VAL:CG1	2.69	0.41
1:A:318:GLY:C	1:A:320:VAL:N	2.78	0.41
1:A:352[A]:GLN:OE1	1:A:416:ARG:HD3	2.20	0.41
1:A:371:ARG:HH21	1:A:375:SER:HB3	1.86	0.41
1:A:122:ASP:HA	1:B:277:VAL:O	2.21	0.41
1:B:42:VAL:HG12	1:B:43:PRO:CD	2.51	0.41
1:B:285:THR:HG23	1:B:287:GLU:H	1.86	0.41
1:B:374:PHE:CZ	1:B:391:ALA:HA	2.56	0.40
1:A:354:ARG:HD3	1:A:354:ARG:HH11	1.72	0.40
1:B:84:ALA:O	1:B:88:ARG:HG2	2.22	0.40
1:A:285:THR:CG2	1:A:288:ALA:H	2.09	0.40
1:B:464:ARG:HB2	1:B:464:ARG:HH11	1.86	0.40
1:B:346:PRO:O	1:B:396:VAL:HG22	2.22	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	529/528 (100%)	507 (96%)	20 (4%)	2 (0%)	30	43
1	B	521/528 (99%)	503 (96%)	15 (3%)	3 (1%)	21	32
All	All	1050/1056 (99%)	1010 (96%)	35 (3%)	5 (0%)	24	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	316	GLY
1	A	319	VAL
1	B	210	THR
1	A	321	ASN
1	B	377	VAL

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	401/398 (101%)	342 (85%)	59 (15%)	3	4
1	B	396/398 (100%)	345 (87%)	51 (13%)	4	6
All	All	797/796 (100%)	687 (86%)	110 (14%)	3	4

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	ILE
1	A	12	LYS
1	A	38	LEU
1	A	39	LEU
1	A	49	LEU
1	A	50	VAL
1	A	51	ARG
1	A	55	THR
1	A	66	LYS
1	A	67	LEU
1	A	69	ILE
1	A	88	ARG
1	A	93	VAL
1	A	110	LEU
1	A	118	ILE
1	A	129	THR
1	A	131	LYS
1	A	152	ARG
1	A	194	LEU
1	A	196	ARG
1	A	202	VAL
1	A	210	THR
1	A	213	LEU
1	A	214	ILE
1	A	219	LEU
1	A	226	VAL
1	A	236	LEU
1	A	242	LEU
1	A	251	VAL
1	A	256	LEU
1	A	261	THR
1	A	274	GLN
1	A	281	LEU
1	A	285	THR
1	A	296	VAL
1	A	328	LEU
1	A	337	LEU
1	A	344	GLU
1	A	345	LEU
1	A	352[A]	GLN
1	A	352[B]	GLN

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Mol	Chain	Res	Type
1	A	371	ARG
1	A	375	SER
1	A	383	THR
1	A	384	PHE
1	A	385	VAL
1	A	418	VAL
1	A	430	THR
1	A	437	SER
1	A	450	LEU
1	A	475	LEU
1	A	487	LEU
1	A	509	ASP
1	A	510	VAL
1	A	523	LEU
1	A	524	GLU
1	A	529	SER
1	B	8	LEU
1	B	18	VAL
1	B	21	LEU
1	B	25	VAL
1	B	42	VAL
1	B	49	LEU
1	B	54	THR
1	B	67	LEU
1	B	88	ARG
1	B	93	VAL
1	B	94	ASN
1	B	99	ASN
1	B	125	LEU
1	B	127	GLU
1	B	161	ILE
1	B	194	LEU
1	B	213	LEU
1	B	216	LYS
1	B	219	LEU
1	B	233	ARG
1	B	269	LEU
1	B	274	GLN
1	B	285	THR
1	B	313	VAL
1	B	315	VAL
1	B	319	VAL

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Mol	Chain	Res	Type
1	B	322	GLU
1	B	330	LEU
1	B	337	LEU
1	B	341	LEU
1	B	342	SER
1	B	343	ASP
1	B	344	GLU
1	B	352	GLN
1	B	357	LEU
1	B	366	ARG
1	B	370	LEU
1	B	373	LEU
1	B	394	ARG
1	B	399	GLU
1	B	408	ASN
1	B	437	SER
1	B	443	ILE
1	B	446	ARG
1	B	464	ARG
1	B	475	LEU
1	B	488	SER
1	B	497	THR
1	B	502	LEU
1	B	522	LYS
1	B	528	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	159	GLN
1	A	230	ASN
1	A	274	GLN
1	A	289	GLN
1	A	409	HIS
1	A	435	GLN
1	A	438	GLN
1	A	504	GLN
1	B	24	GLN
1	B	94	ASN
1	B	99	ASN
1	B	117	GLN
1	B	155	GLN

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Mol	Chain	Res	Type
1	B	274	GLN
1	B	289	GLN
1	B	352	GLN
1	B	408	ASN
1	B	409	HIS

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	TLA	B	530	-	9,9,9	0.96	1 (11%)	12,12,12	1.34	2 (16%)
2	TLA	A	530	-	9,9,9	0.85	1 (11%)	12,12,12	1.81	3 (25%)
2	TLA	B	531	-	9,9,9	1.01	0	12,12,12	1.34	1 (8%)
3	HPV	B	600	-	10,10,10	1.80	1 (10%)	12,14,14	2.25	2 (16%)

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	TLA	B	530	-	-	0/12/12/12	-
2	TLA	A	530	-	-	0/12/12/12	-
2	TLA	B	531	-	-	2/12/12/12	-
3	HPV	B	600	-	-	7/9/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	HPV	C2-C1	-5.16	1.45	1.53
2	B	530	TLA	C3-C4	-2.14	1.49	1.52
2	A	530	TLA	C2-C1	-2.11	1.49	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	HPV	O1-C1-C2	-6.41	113.84	121.81
2	A	530	TLA	O41-C4-C3	3.27	122.39	113.31
2	A	530	TLA	O11-C1-C2	3.15	122.07	113.31
3	B	600	HPV	O2-C1-C2	2.91	121.65	113.59
2	B	530	TLA	O11-C1-C2	2.85	121.24	113.31
2	A	530	TLA	O41-C4-O4	-2.79	117.74	124.08
2	B	531	TLA	O41-C4-C3	2.76	120.98	113.31
2	B	530	TLA	O11-C1-O1	-2.22	119.05	124.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	600	HPV	O1-C1-C2-C3
3	B	600	HPV	O1-C1-C2-O3
3	B	600	HPV	C3-O1P-P-O4P
3	B	600	HPV	C3-O1P-P-O2P
3	B	600	HPV	C3-O1P-P-O3P
3	B	600	HPV	C1-C2-C3-O1P
3	B	600	HPV	O3-C2-C3-O1P
2	B	531	TLA	C2-C3-C4-O4
2	B	531	TLA	C2-C3-C4-O41

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	530	TLA	1	0
3	B	600	HPV	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

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	527/528 (99%)	0.26	13 (2%) 58 54	22, 40, 64, 85	6 (1%)
1	B	525/528 (99%)	0.34	28 (5%) 32 28	26, 40, 63, 85	22 (4%)
All	All	1052/1056 (99%)	0.30	41 (3%) 43 39	22, 40, 64, 85	28 (2%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	SER	12.3
1	B	385	VAL	9.1
1	B	382	VAL	7.9
1	B	211	ALA	7.4
1	B	379	GLU	6.4
1	A	492	GLU	6.1
1	B	210	THR	6.0
1	B	383	THR	5.9
1	B	384	PHE	5.8
1	B	378	ILE	5.6
1	B	377	VAL	5.1
1	B	386	ASN	4.6
1	B	209	GLU	4.5
1	A	319	VAL	4.4
1	B	392	ALA	4.3
1	A	167[A]	TYR	3.9
1	B	388	PRO	3.9
1	B	319	VAL	3.7
1	A	206	LYS	3.5
1	A	381	ALA	3.5
1	B	317	GLY	3.5
1	B	315	VAL	3.5
1	B	316	GLY	3.5
1	B	318	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	389	ALA	3.3
1	B	491	ALA	3.1
1	A	384	PHE	3.0
1	B	41	ALA	2.9
1	B	213	LEU	2.9
1	B	212	GLY	2.7
1	A	385	VAL	2.7
1	B	390	LEU	2.6
1	A	491	ALA	2.6
1	A	318	GLY	2.5
1	B	529	SER	2.5
1	A	382	VAL	2.5
1	A	308	PHE	2.4
1	B	65	PRO	2.4
1	B	391	ALA	2.3
1	B	3	SER	2.3
1	A	315	VAL	2.1

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
3	HPV	B	600	11/11	0.83	0.24	28,43,61,63	11
2	TLA	A	530	10/10	0.93	0.09	36,42,49,54	0
2	TLA	B	531	10/10	0.94	0.16	22,33,36,40	10
2	TLA	B	530	10/10	0.95	0.13	30,36,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.