



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:07 PM UTC

PDB ID : 3GOY / pdb_00003goy
Title : Crystal structure of human poly(adp-ribose) polymerase 14, catalytic fragment in complex with an inhibitor 3-aminobenzamide
Authors : Karlberg, T.; Moche, M.; Lehtio, L.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Kotenyova, T.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Schutz, P.; Siponen, M.I.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Wisniewska, M.; Schuler, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-03-20
Resolution : 2.80 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

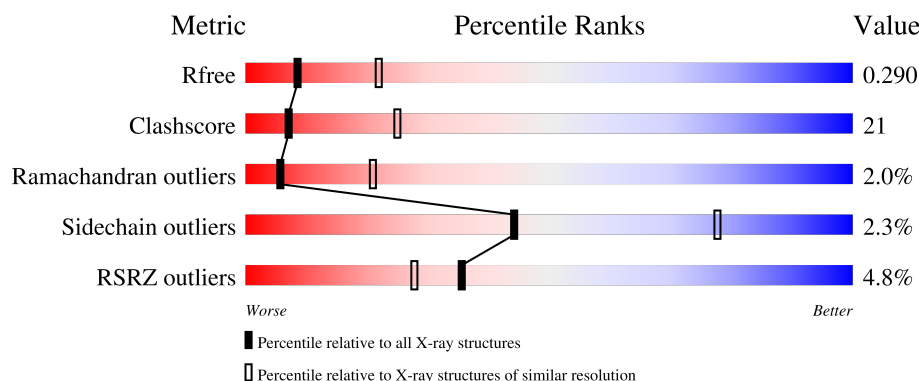
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	193	
1	B	193	
1	C	193	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	193	6% 58% 34% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5834 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.

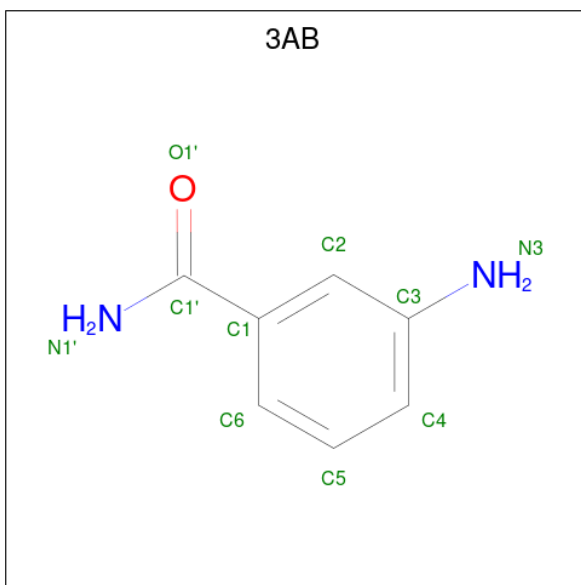
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1448	916	252	276	4			
1	B	181	Total	C	N	O	S	0	0	0
			1450	919	250	277	4			
1	C	181	Total	C	N	O	S	0	0	0
			1442	915	246	277	4			
1	D	182	Total	C	N	O	S	0	0	0
			1454	922	250	278	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1528	SER	-	expression tag	UNP Q460N5
A	1529	MET	-	expression tag	UNP Q460N5
B	1528	SER	-	expression tag	UNP Q460N5
B	1529	MET	-	expression tag	UNP Q460N5
C	1528	SER	-	expression tag	UNP Q460N5
C	1529	MET	-	expression tag	UNP Q460N5
D	1528	SER	-	expression tag	UNP Q460N5
D	1529	MET	-	expression tag	UNP Q460N5

- Molecule 2 is 3-aminobenzamide (CCD ID: 3AB) (formula: C₇H₈N₂O).

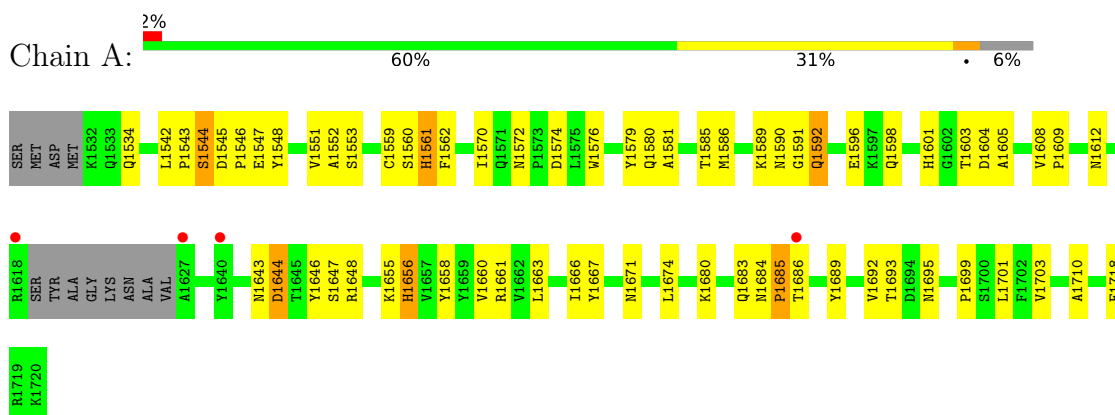


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	2	1		
2	B	1	Total	C	N	O	0	0
			10	7	2	1		
2	C	1	Total	C	N	O	0	0
			10	7	2	1		
2	D	1	Total	C	N	O	0	0
			10	7	2	1		

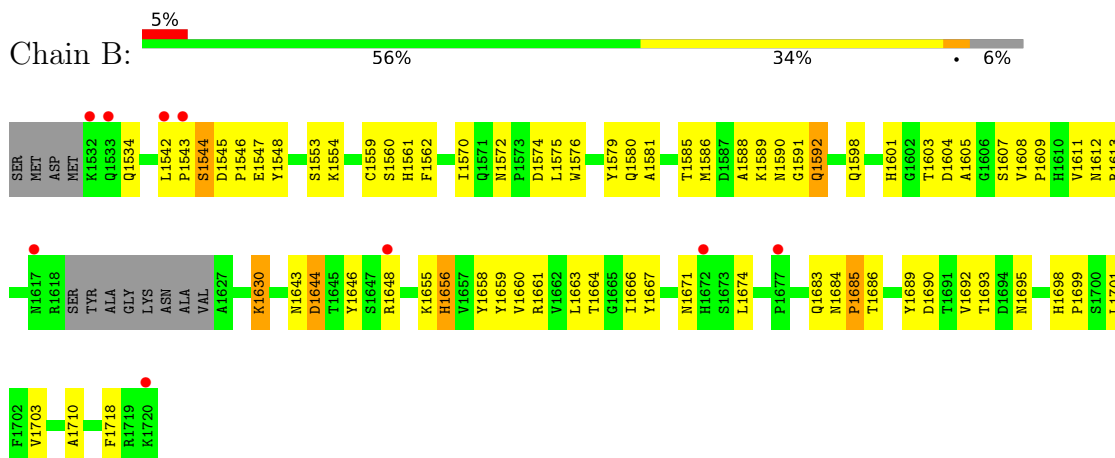
3 Residue-property plots

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.

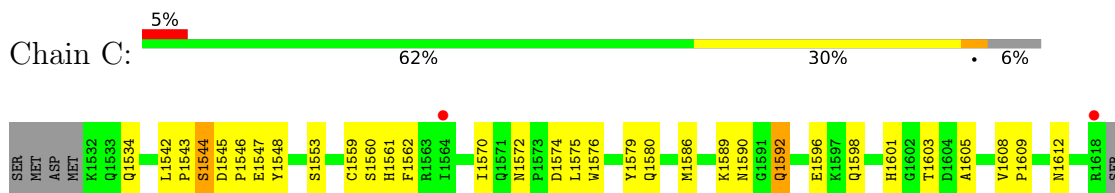
- Molecule 1: Poly [ADP-ribose] polymerase 14

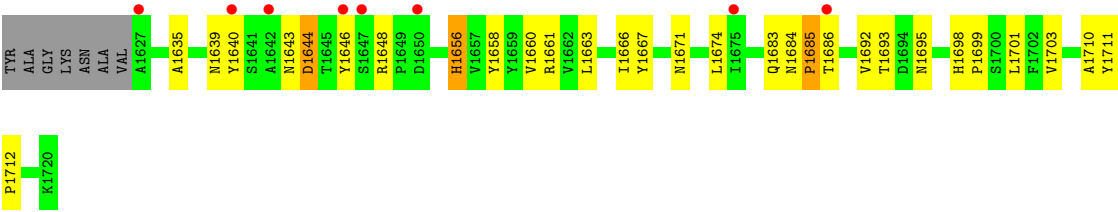


- Molecule 1: Poly [ADP-ribose] polymerase 14

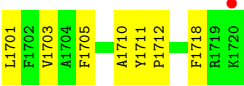
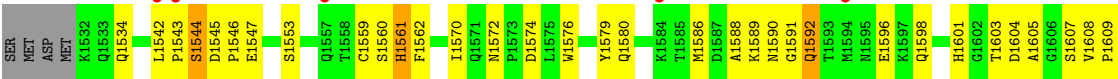


- Molecule 1: Poly [ADP-ribose] polymerase 14





● Molecule 1: Poly [ADP-ribose] polymerase 14



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.75Å 144.27Å 79.70Å 90.00° 100.55° 90.00°	Depositor
Resolution (Å)	24.56 – 2.80 24.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (24.56-2.80) 98.8 (24.56-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.253 , 0.292 0.253 , 0.290	Depositor DCC
R_{free} test set	1119 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 108.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5834	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3422e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 3AB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/1489	0.85	0/2028
1	B	0.53	0/1492	0.88	0/2033
1	C	0.44	0/1484	0.85	0/2024
1	D	0.48	0/1496	0.86	1/2040 (0.0%)
All	All	0.49	0/5961	0.86	1/8125 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1645	THR	N-CA-C	-5.75	105.76	112.89

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	1448	0	1333	64	0
1	B	1450	0	1346	66	0
1	C	1442	0	1328	57	0
1	D	1454	0	1346	63	0
2	A	10	0	8	2	0
2	B	10	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	8	1	0
2	D	10	0	8	0	0
All	All	5834	0	5385	234	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 21.

All (234) 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:1592:GLN:HG2	1:D:1667:TYR:CZ	1.99	0.96
1:A:1534:GLN:HB3	1:A:1572:ASN:HD21	1.38	0.88
1:D:1534:GLN:HB3	1:D:1572:ASN:HD21	1.39	0.86
1:A:1592:GLN:HG2	1:C:1667:TYR:CZ	2.10	0.85
1:A:1592:GLN:HG2	1:C:1667:TYR:CE1	2.12	0.84
1:A:1551:VAL:C	1:A:1552:ALA:CA	2.53	0.81
1:B:1554:LYS:HD2	1:B:1659:TYR:OH	1.82	0.78
1:A:1701:LEU:HD22	2:A:1:3AB:H4	1.67	0.77
1:A:1667:TYR:CE1	1:C:1592:GLN:HG2	2.19	0.76
1:D:1693:THR:OG1	1:D:1699:PRO:HB3	1.85	0.76
1:B:1534:GLN:HB3	1:B:1572:ASN:HD21	1.52	0.75
1:C:1693:THR:OG1	1:C:1699:PRO:HB3	1.86	0.75
1:B:1592:GLN:HG2	1:D:1667:TYR:CE1	2.21	0.74
1:A:1667:TYR:CZ	1:C:1592:GLN:HG2	2.22	0.74
1:B:1693:THR:OG1	1:B:1699:PRO:HB3	1.89	0.72
1:A:1572:ASN:OD1	1:A:1572:ASN:C	2.34	0.71
1:B:1666:ILE:HA	1:D:1592:GLN:OE1	1.90	0.71
1:B:1667:TYR:CZ	1:D:1592:GLN:HG2	2.25	0.70
1:B:1572:ASN:C	1:B:1572:ASN:OD1	2.34	0.70
1:A:1589:LYS:HE3	1:A:1590:ASN:OD1	1.91	0.70
1:B:1589:LYS:HE3	1:B:1590:ASN:OD1	1.92	0.69
1:C:1605:ALA:HB2	1:C:1656:HIS:NE2	2.09	0.68
1:B:1667:TYR:CE1	1:D:1592:GLN:HG2	2.29	0.67
1:A:1693:THR:OG1	1:A:1699:PRO:HB3	1.94	0.67
1:B:1661:ARG:O	1:B:1710:ALA:HA	1.95	0.67
1:D:1661:ARG:O	1:D:1710:ALA:HA	1.95	0.66
1:A:1661:ARG:O	1:A:1710:ALA:HA	1.95	0.65
1:D:1655:LYS:HE3	1:D:1718:PHE:CE1	2.31	0.64
1:C:1661:ARG:O	1:C:1710:ALA:HA	1.98	0.64
1:B:1542:LEU:HD12	1:B:1543:PRO:HD2	1.79	0.64
1:C:1589:LYS:HE3	1:C:1590:ASN:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1605:ALA:HB2	1:D:1656:HIS:NE2	2.13	0.64
1:D:1570:ILE:HD13	1:D:1612:ASN:ND2	2.13	0.64
1:D:1589:LYS:HE3	1:D:1590:ASN:OD1	1.97	0.63
1:A:1542:LEU:HD12	1:A:1543:PRO:HD2	1.81	0.63
1:C:1570:ILE:HD13	1:C:1612:ASN:ND2	2.13	0.62
1:A:1570:ILE:HD13	1:A:1612:ASN:ND2	2.15	0.62
1:C:1542:LEU:HD12	1:C:1543:PRO:HD2	1.80	0.62
1:A:1605:ALA:HB2	1:A:1656:HIS:NE2	2.14	0.61
1:B:1570:ILE:HD13	1:B:1612:ASN:ND2	2.15	0.61
1:B:1534:GLN:HG2	1:B:1574:ASP:HB2	1.83	0.61
1:B:1605:ALA:HB2	1:B:1656:HIS:NE2	2.15	0.61
1:D:1542:LEU:HD12	1:D:1543:PRO:HD2	1.82	0.60
1:C:1534:GLN:HG2	1:C:1574:ASP:HB2	1.83	0.60
1:B:1601:HIS:NE2	1:B:1603:THR:HG23	2.16	0.60
1:B:1655:LYS:HE3	1:B:1718:PHE:CE1	2.38	0.59
1:A:1655:LYS:HE3	1:A:1718:PHE:CE1	2.38	0.59
1:A:1534:GLN:HG2	1:A:1574:ASP:HB2	1.86	0.58
1:C:1601:HIS:NE2	1:C:1603:THR:HG23	2.17	0.58
1:B:1630:LYS:HB2	1:B:1630:LYS:NZ	2.19	0.58
1:D:1671:ASN:H	1:D:1674:LEU:CD1	2.16	0.58
1:C:1701:LEU:HD12	1:C:1701:LEU:C	2.29	0.58
1:D:1534:GLN:HG2	1:D:1574:ASP:HB2	1.86	0.57
1:B:1534:GLN:HG2	1:B:1574:ASP:CB	2.35	0.57
1:D:1601:HIS:NE2	1:D:1603:THR:HG23	2.19	0.57
1:D:1534:GLN:HG2	1:D:1574:ASP:CB	2.35	0.57
1:A:1671:ASN:H	1:A:1674:LEU:CD1	2.18	0.56
1:D:1579:TYR:HE1	1:D:1663:LEU:HG	1.69	0.56
1:A:1601:HIS:NE2	1:A:1603:THR:HG23	2.20	0.56
1:A:1534:GLN:HG2	1:A:1574:ASP:CB	2.36	0.56
1:D:1534:GLN:O	1:D:1572:ASN:ND2	2.39	0.56
1:A:1701:LEU:C	1:A:1701:LEU:HD12	2.31	0.56
1:D:1586:MET:HE1	1:D:1663:LEU:HB3	1.87	0.56
1:D:1701:LEU:C	1:D:1701:LEU:HD12	2.31	0.55
1:C:1534:GLN:HG2	1:C:1574:ASP:CB	2.36	0.55
1:B:1543:PRO:O	1:B:1544:SER:CB	2.55	0.55
1:C:1543:PRO:O	1:C:1544:SER:CB	2.54	0.55
1:A:1543:PRO:O	1:A:1544:SER:CB	2.55	0.55
1:B:1671:ASN:H	1:B:1674:LEU:CD1	2.20	0.55
1:C:1561:HIS:CE1	1:C:1562:PHE:CE2	2.96	0.54
1:D:1543:PRO:O	1:D:1544:SER:CB	2.55	0.54
1:D:1560:SER:C	1:D:1562:PHE:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1561:HIS:CE1	1:D:1562:PHE:CE2	2.96	0.54
1:B:1576:TRP:O	1:B:1580:GLN:HG2	2.08	0.54
1:A:1543:PRO:O	1:A:1544:SER:HB2	2.07	0.54
1:B:1592:GLN:HG2	1:D:1667:TYR:CE2	2.42	0.54
1:B:1579:TYR:HE1	1:B:1663:LEU:HG	1.72	0.53
1:A:1666:ILE:HA	1:C:1592:GLN:OE1	2.07	0.53
1:D:1576:TRP:O	1:D:1580:GLN:HG2	2.09	0.53
1:A:1560:SER:C	1:A:1562:PHE:H	2.16	0.53
1:B:1701:LEU:C	1:B:1701:LEU:HD12	2.33	0.53
1:C:1546:PRO:HG2	1:C:1547:GLU:H	1.74	0.53
1:A:1586:MET:HE1	1:A:1663:LEU:HB3	1.90	0.53
1:D:1579:TYR:CE1	1:D:1663:LEU:HG	2.44	0.53
1:B:1588:ALA:O	1:D:1689:TYR:OH	2.26	0.53
1:C:1543:PRO:O	1:C:1544:SER:HB2	2.09	0.53
1:C:1560:SER:C	1:C:1562:PHE:H	2.16	0.52
1:C:1671:ASN:H	1:C:1674:LEU:CD1	2.21	0.52
1:C:1598:GLN:HA	1:C:1660:VAL:O	2.10	0.52
1:B:1543:PRO:O	1:B:1544:SER:HB2	2.09	0.52
1:C:1586:MET:HE1	1:C:1663:LEU:HB3	1.90	0.52
1:A:1579:TYR:HE1	1:A:1663:LEU:HG	1.73	0.52
1:A:1701:LEU:HB2	2:A:1:3AB:H5	1.91	0.51
1:B:1560:SER:C	1:B:1562:PHE:H	2.17	0.51
1:B:1586:MET:HE1	1:B:1663:LEU:HB3	1.92	0.51
1:B:1611:VAL:HB	1:B:1658:TYR:HH	1.76	0.51
1:D:1543:PRO:O	1:D:1544:SER:HB2	2.10	0.51
1:C:1643:ASN:HB2	1:C:1646:TYR:CD2	2.45	0.51
1:A:1579:TYR:CE1	1:A:1663:LEU:HG	2.46	0.51
1:C:1684:ASN:C	1:C:1686:THR:H	2.19	0.51
1:A:1576:TRP:O	1:A:1580:GLN:HG2	2.11	0.51
1:B:1561:HIS:CE1	1:B:1562:PHE:CE2	2.98	0.51
1:D:1684:ASN:C	1:D:1686:THR:H	2.19	0.51
1:A:1561:HIS:CE1	1:A:1562:PHE:CE2	2.98	0.50
1:B:1598:GLN:HA	1:B:1660:VAL:O	2.11	0.50
1:C:1579:TYR:HE1	1:C:1663:LEU:HG	1.75	0.50
1:D:1546:PRO:HG2	1:D:1547:GLU:H	1.77	0.50
1:D:1612:ASN:ND2	1:D:1658:TYR:OH	2.44	0.50
1:A:1684:ASN:C	1:A:1686:THR:H	2.18	0.50
1:D:1598:GLN:HA	1:D:1660:VAL:O	2.11	0.50
1:B:1684:ASN:C	1:B:1686:THR:H	2.19	0.50
1:A:1572:ASN:OD1	1:A:1572:ASN:O	2.30	0.50
1:A:1534:GLN:O	1:A:1572:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1572:ASN:OD1	1:B:1572:ASN:O	2.29	0.49
1:C:1579:TYR:CE1	1:C:1663:LEU:HG	2.47	0.49
1:A:1592:GLN:OE1	1:C:1666:ILE:HA	2.12	0.49
1:A:1671:ASN:H	1:A:1674:LEU:HD11	1.78	0.49
1:A:1643:ASN:HB2	1:A:1646:TYR:CD2	2.47	0.49
1:A:1546:PRO:HG2	1:A:1547:GLU:H	1.78	0.49
1:D:1643:ASN:HB2	1:D:1646:TYR:CD2	2.47	0.49
1:D:1586:MET:HG2	1:D:1590:ASN:ND2	2.28	0.49
1:D:1671:ASN:H	1:D:1674:LEU:HD11	1.77	0.48
1:B:1579:TYR:CE1	1:B:1663:LEU:HG	2.48	0.48
1:A:1701:LEU:HD12	1:A:1701:LEU:O	2.14	0.48
1:D:1576:TRP:CZ2	1:D:1580:GLN:NE2	2.80	0.48
1:B:1692:VAL:HG23	1:B:1703:VAL:HB	1.95	0.48
1:B:1546:PRO:HG2	1:B:1547:GLU:H	1.79	0.48
1:A:1576:TRP:CZ2	1:A:1580:GLN:NE2	2.82	0.48
1:C:1644:ASP:OD1	1:C:1644:ASP:N	2.46	0.48
1:B:1612:ASN:ND2	1:B:1658:TYR:OH	2.47	0.48
1:A:1612:ASN:ND2	1:A:1658:TYR:OH	2.47	0.47
1:C:1576:TRP:O	1:C:1580:GLN:HG2	2.14	0.47
1:A:1644:ASP:N	1:A:1644:ASP:OD1	2.46	0.47
1:D:1644:ASP:N	1:D:1644:ASP:OD1	2.47	0.47
1:B:1644:ASP:OD1	1:B:1644:ASP:N	2.47	0.47
1:C:1701:LEU:HD12	1:C:1701:LEU:O	2.14	0.46
1:A:1598:GLN:HA	1:A:1660:VAL:O	2.15	0.46
1:D:1695:ASN:OD1	1:D:1695:ASN:C	2.58	0.46
1:D:1572:ASN:OD1	1:D:1572:ASN:C	2.58	0.46
1:C:1612:ASN:ND2	1:C:1658:TYR:OH	2.48	0.46
1:C:1635:ALA:HB2	2:C:1:3AB:H6	1.97	0.46
1:B:1586:MET:HG2	1:B:1590:ASN:ND2	2.31	0.46
1:B:1689:TYR:OH	1:D:1588:ALA:O	2.33	0.46
1:A:1581:ALA:O	1:A:1585:THR:HG23	2.15	0.46
1:A:1608:VAL:HB	1:A:1609:PRO:HD3	1.98	0.46
1:B:1643:ASN:HB2	1:B:1646:TYR:CD2	2.50	0.46
1:D:1626:VAL:HB	1:D:1629:GLY:O	2.14	0.46
1:C:1586:MET:HG2	1:C:1590:ASN:ND2	2.30	0.46
1:A:1559:CYS:HB3	1:A:1562:PHE:CD2	2.51	0.46
1:A:1648:ARG:CZ	1:A:1648:ARG:HB3	2.47	0.46
1:B:1701:LEU:HD12	1:B:1701:LEU:O	2.16	0.45
1:A:1586:MET:HG2	1:A:1590:ASN:ND2	2.32	0.45
1:A:1542:LEU:O	1:A:1545:ASP:HB2	2.17	0.45
1:B:1590:ASN:O	1:B:1591:GLY:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1576:TRP:CZ2	1:C:1580:GLN:NE2	2.83	0.45
1:B:1576:TRP:CZ2	1:B:1580:GLN:NE2	2.83	0.45
1:B:1648:ARG:CZ	1:B:1648:ARG:HB3	2.47	0.45
1:C:1575:LEU:HD23	1:C:1575:LEU:HA	1.87	0.45
1:C:1608:VAL:HB	1:C:1609:PRO:HD3	1.98	0.45
1:D:1542:LEU:O	1:D:1545:ASP:HB2	2.17	0.44
1:D:1692:VAL:HG23	1:D:1703:VAL:HB	1.98	0.44
1:C:1542:LEU:O	1:C:1545:ASP:HB2	2.17	0.44
1:C:1559:CYS:O	1:C:1562:PHE:HB2	2.17	0.44
1:B:1671:ASN:H	1:B:1674:LEU:HD11	1.83	0.44
1:C:1698:HIS:N	1:C:1699:PRO:HD3	2.32	0.44
1:D:1683:GLN:C	1:D:1685:PRO:HD3	2.43	0.44
1:B:1542:LEU:O	1:B:1545:ASP:HB2	2.18	0.44
1:C:1559:CYS:HB3	1:C:1562:PHE:CD2	2.52	0.44
1:C:1695:ASN:C	1:C:1695:ASN:OD1	2.60	0.44
1:C:1711:TYR:HA	1:C:1712:PRO:HD3	1.84	0.44
1:A:1608:VAL:HA	1:A:1658:TYR:HH	1.82	0.44
1:A:1692:VAL:HG23	1:A:1703:VAL:HB	2.00	0.43
1:A:1592:GLN:HG2	1:C:1667:TYR:CE2	2.52	0.43
1:C:1648:ARG:CZ	1:C:1648:ARG:HB3	2.47	0.43
1:D:1639:ASN:OD1	1:D:1640:TYR:N	2.51	0.43
1:D:1590:ASN:O	1:D:1591:GLY:C	2.59	0.43
1:D:1592:GLN:H	1:D:1592:GLN:HG3	1.37	0.43
1:B:1561:HIS:H	1:B:1561:HIS:CD2	2.36	0.43
1:D:1559:CYS:O	1:D:1562:PHE:HB2	2.18	0.43
1:C:1592:GLN:H	1:C:1592:GLN:HG3	1.40	0.43
1:D:1711:TYR:HA	1:D:1712:PRO:HD3	1.83	0.43
1:B:1684:ASN:CG	1:B:1684:ASN:O	2.62	0.43
1:C:1692:VAL:HG23	1:C:1703:VAL:HB	1.99	0.43
1:B:1575:LEU:HD23	1:B:1575:LEU:HA	1.88	0.43
1:C:1561:HIS:CD2	1:C:1561:HIS:H	2.37	0.43
1:C:1683:GLN:C	1:C:1685:PRO:HD3	2.44	0.43
1:D:1534:GLN:HG2	1:D:1574:ASP:HB3	2.01	0.43
1:C:1639:ASN:OD1	1:C:1640:TYR:N	2.52	0.42
1:D:1561:HIS:CD2	1:D:1561:HIS:H	2.36	0.42
1:D:1684:ASN:CG	1:D:1684:ASN:O	2.62	0.42
1:A:1590:ASN:O	1:A:1591:GLY:C	2.61	0.42
1:B:1559:CYS:O	1:B:1562:PHE:HB2	2.19	0.42
1:B:1695:ASN:OD1	1:B:1695:ASN:C	2.61	0.42
1:A:1695:ASN:C	1:A:1695:ASN:OD1	2.60	0.42
1:A:1684:ASN:O	1:A:1684:ASN:CG	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1581:ALA:O	1:B:1585:THR:HG23	2.20	0.42
1:D:1648:ARG:CZ	1:D:1648:ARG:HB3	2.49	0.42
1:B:1608:VAL:HB	1:B:1609:PRO:HD3	2.02	0.42
1:C:1579:TYR:OH	1:C:1596:GLU:HG3	2.20	0.42
1:C:1570:ILE:CD1	1:C:1612:ASN:ND2	2.82	0.42
1:A:1683:GLN:C	1:A:1685:PRO:HD3	2.44	0.42
1:B:1548:TYR:CD2	1:B:1548:TYR:C	2.98	0.42
1:B:1683:GLN:C	1:B:1685:PRO:HD3	2.45	0.42
1:D:1692:VAL:HG22	1:D:1705:PHE:HE2	1.85	0.42
1:A:1559:CYS:O	1:A:1562:PHE:HB2	2.19	0.41
1:D:1579:TYR:OH	1:D:1596:GLU:HG3	2.20	0.41
1:C:1548:TYR:C	1:C:1548:TYR:CD2	2.98	0.41
1:A:1680:LYS:HA	1:A:1689:TYR:CE2	2.56	0.41
1:D:1608:VAL:HB	1:D:1609:PRO:HD3	2.02	0.41
1:D:1693:THR:HG1	1:D:1699:PRO:HB3	1.82	0.41
1:A:1561:HIS:CD2	1:A:1561:HIS:H	2.37	0.41
1:B:1698:HIS:N	1:B:1699:PRO:HD3	2.35	0.41
1:D:1604:ASP:OD1	1:D:1607:SER:N	2.51	0.41
1:B:1664:THR:O	1:B:1690:ASP:HB2	2.20	0.41
1:C:1684:ASN:O	1:C:1684:ASN:CG	2.63	0.41
1:A:1548:TYR:CD2	1:A:1548:TYR:C	2.99	0.41
1:A:1579:TYR:OH	1:A:1596:GLU:HG3	2.20	0.41
1:B:1613:ARG:HE	1:B:1613:ARG:HB2	1.70	0.41
1:B:1693:THR:HG1	1:B:1699:PRO:HB3	1.85	0.41
1:C:1572:ASN:HB3	1:C:1575:LEU:HB2	2.03	0.41
1:D:1570:ILE:CD1	1:D:1612:ASN:ND2	2.82	0.41
1:D:1698:HIS:N	1:D:1699:PRO:HD3	2.35	0.41
1:A:1667:TYR:CD1	1:C:1592:GLN:HG2	2.56	0.41
1:B:1592:GLN:H	1:B:1592:GLN:HG3	1.34	0.41
1:D:1701:LEU:HD12	1:D:1701:LEU:O	2.20	0.41
1:B:1666:ILE:HG22	1:B:1689:TYR:HD1	1.86	0.40
1:C:1660:VAL:CG1	1:C:1710:ALA:HB1	2.51	0.40
1:A:1604:ASP:OD1	1:A:1604:ASP:C	2.64	0.40
1:B:1554:LYS:HD2	1:B:1659:TYR:CZ	2.56	0.40
1:B:1604:ASP:OD1	1:B:1607:SER:N	2.54	0.40
1:D:1664:THR:O	1:D:1690:ASP:HB2	2.22	0.40
1:A:1693:THR:HG1	1:A:1699:PRO:HB3	1.86	0.40
1:A:1559:CYS:HB3	1:A:1562:PHE:HD2	1.87	0.40
1:B:1554:LYS:CD	1:B:1659:TYR:OH	2.63	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	175/193 (91%)	155 (89%)	16 (9%)	4 (2%)	5	18
1	B	177/193 (92%)	159 (90%)	15 (8%)	3 (2%)	7	25
1	C	177/193 (92%)	159 (90%)	15 (8%)	3 (2%)	7	25
1	D	178/193 (92%)	157 (88%)	17 (10%)	4 (2%)	5	19
All	All	707/772 (92%)	630 (89%)	63 (9%)	14 (2%)	6	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1544	SER
1	B	1544	SER
1	C	1544	SER
1	D	1544	SER
1	B	1553	SER
1	C	1553	SER
1	D	1553	SER
1	D	1561	HIS
1	A	1553	SER
1	A	1561	HIS
1	A	1685	PRO
1	D	1685	PRO
1	B	1685	PRO
1	C	1685	PRO

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	155/170 (91%)	151 (97%)	4 (3%)	40	75
1	B	156/170 (92%)	152 (97%)	4 (3%)	40	75
1	C	154/170 (91%)	151 (98%)	3 (2%)	50	81
1	D	156/170 (92%)	153 (98%)	3 (2%)	50	81
All	All	621/680 (91%)	607 (98%)	14 (2%)	44	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1592	GLN
1	A	1644	ASP
1	A	1647	SER
1	A	1656	HIS
1	B	1592	GLN
1	B	1630	LYS
1	B	1644	ASP
1	B	1656	HIS
1	C	1592	GLN
1	C	1644	ASP
1	C	1656	HIS
1	D	1592	GLN
1	D	1644	ASP
1	D	1656	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1534	GLN
1	A	1561	HIS
1	A	1571	GLN
1	A	1612	ASN
1	A	1671	ASN
1	B	1534	GLN
1	B	1561	HIS
1	B	1571	GLN
1	B	1612	ASN
1	B	1671	ASN
1	B	1683	GLN
1	C	1534	GLN
1	C	1561	HIS

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Mol	Chain	Res	Type
1	C	1612	ASN
1	C	1671	ASN
1	C	1683	GLN
1	D	1534	GLN
1	D	1561	HIS
1	D	1612	ASN
1	D	1671	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 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	3AB	B	1	-	10,10,10	0.76	0	13,13,13	1.23	1 (7%)
2	3AB	D	1	-	10,10,10	0.65	0	13,13,13	1.44	2 (15%)
2	3AB	A	1	-	10,10,10	1.71	1 (10%)	13,13,13	1.57	3 (23%)
2	3AB	C	1	-	10,10,10	0.76	0	13,13,13	1.12	1 (7%)

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	3AB	B	1	-	-	0/4/4/4	0/1/1/1
2	3AB	D	1	-	-	0/4/4/4	0/1/1/1
2	3AB	A	1	-	-	0/4/4/4	0/1/1/1
2	3AB	C	1	-	-	0/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	3AB	C6-C1	-2.51	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	3AB	C1-C1'-N1'	-3.58	113.33	117.74
2	B	1	3AB	C1-C1'-N1'	-3.29	113.68	117.74
2	C	1	3AB	C1-C1'-N1'	-2.82	114.27	117.74
2	A	1	3AB	C1-C1'-N1'	-2.69	114.43	117.74
2	A	1	3AB	C1-C2-C3	-2.68	118.45	120.66
2	D	1	3AB	O1'-C1'-N1'	2.15	125.72	122.62
2	A	1	3AB	C6-C1-C2	2.07	121.64	119.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	3AB	2	0
2	C	1	3AB	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	181/193 (93%)	0.35	4 (2%) 62 52	61, 75, 123, 179	0
1	B	181/193 (93%)	0.49	9 (4%) 34 26	27, 63, 122, 178	0
1	C	181/193 (93%)	0.63	10 (5%) 30 23	67, 86, 130, 180	0
1	D	182/193 (94%)	0.45	12 (6%) 24 18	33, 67, 124, 179	0
All	All	725/772 (93%)	0.48	35 (4%) 35 28	27, 75, 130, 180	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1627	ALA	4.4
1	A	1686	THR	3.5
1	B	1720	LYS	3.5
1	B	1672	HIS	3.2
1	B	1533	GLN	3.1
1	B	1543	PRO	3.1
1	C	1642	ALA	2.9
1	D	1618	ARG	2.9
1	C	1618	ARG	2.7
1	C	1646	TYR	2.6
1	D	1542	LEU	2.5
1	D	1675	ILE	2.5
1	C	1675	ILE	2.5
1	D	1626	VAL	2.5
1	B	1542	LEU	2.4
1	B	1648	ARG	2.4
1	D	1648	ARG	2.4
1	D	1557	GLN	2.4
1	D	1684	ASN	2.3
1	D	1720	LYS	2.3
1	D	1594	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1647	SER	2.3
1	B	1617	ASN	2.2
1	A	1627	ALA	2.2
1	C	1564	ILE	2.2
1	C	1686	THR	2.2
1	C	1650	ASP	2.2
1	B	1532	LYS	2.2
1	B	1677	PRO	2.1
1	C	1640	TYR	2.1
1	D	1543	PRO	2.1
1	A	1640	TYR	2.1
1	D	1687	ASP	2.1
1	A	1618	ARG	2.0
1	D	1584	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	3AB	C	1	10/10	0.84	0.13	48,74,88,91	0
2	3AB	D	1	10/10	0.90	0.13	39,58,80,85	0
2	3AB	B	1	10/10	0.92	0.12	17,47,83,93	0
2	3AB	A	1	10/10	0.95	0.08	10,25,49,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.