



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:36 am GMT

PDB ID : 3GOY  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

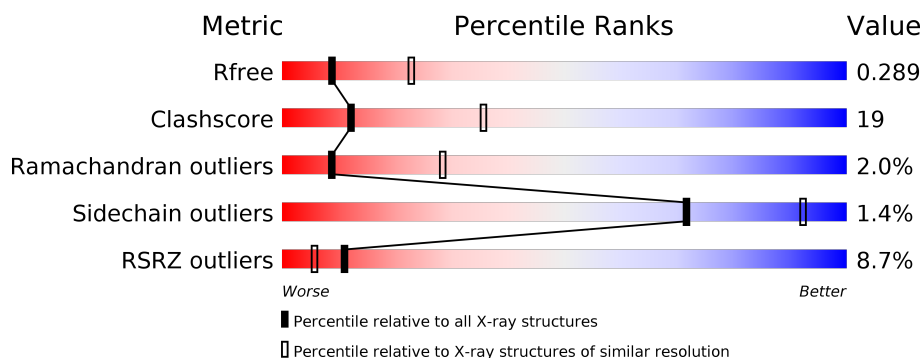
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	193	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>29%</div> <div>6%</div> </div> </div>
1	B	193	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>33%</div> <div>6%</div> </div> </div>
1	C	193	<div> <div>11%</div> <div> <div></div> <div>63%</div> <div>29%</div> <div>6%</div> </div> </div>
1	D	193	<div> <div>9%</div> <div> <div></div> <div>59%</div> <div>34%</div> <div>6%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3AB	D	1	-	-	-	X

## 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.

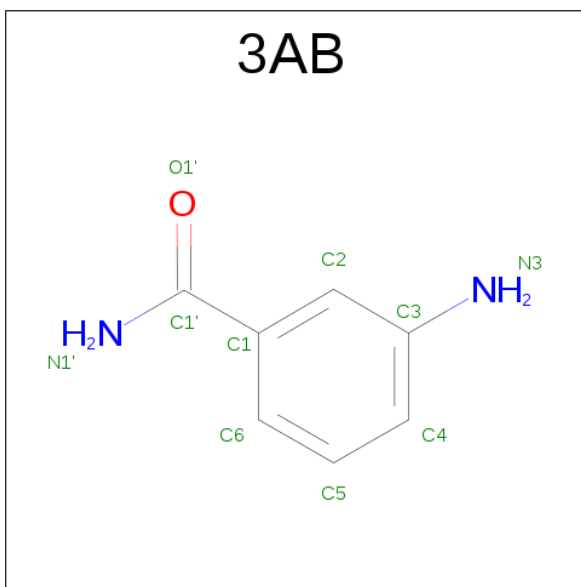
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 14.

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 (three-letter code: 3AB) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O).

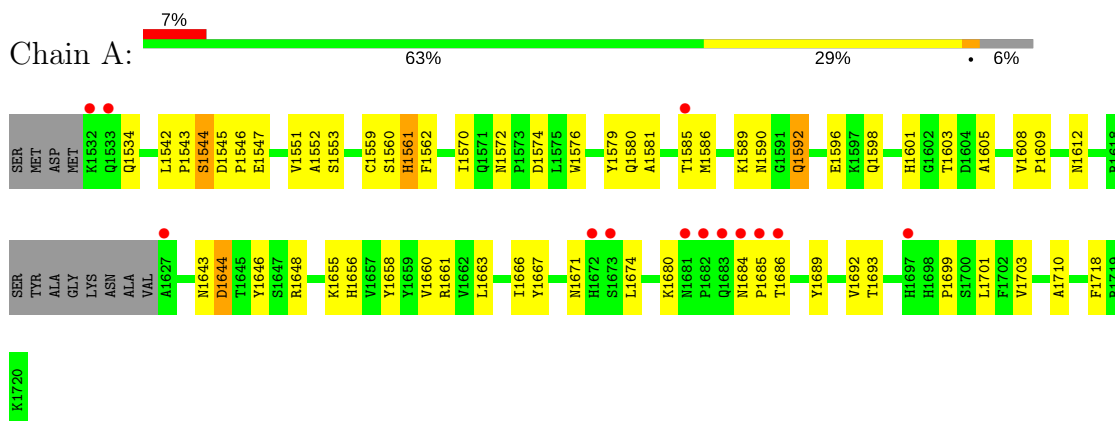


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	2	1		
2	B	1	Total	C	N	O	0	0
			10	7	2	1		
2	C	1	Total	C	N	O	0	0
			10	7	2	1		
2	D	1	Total	C	N	O	0	0
			10	7	2	1		

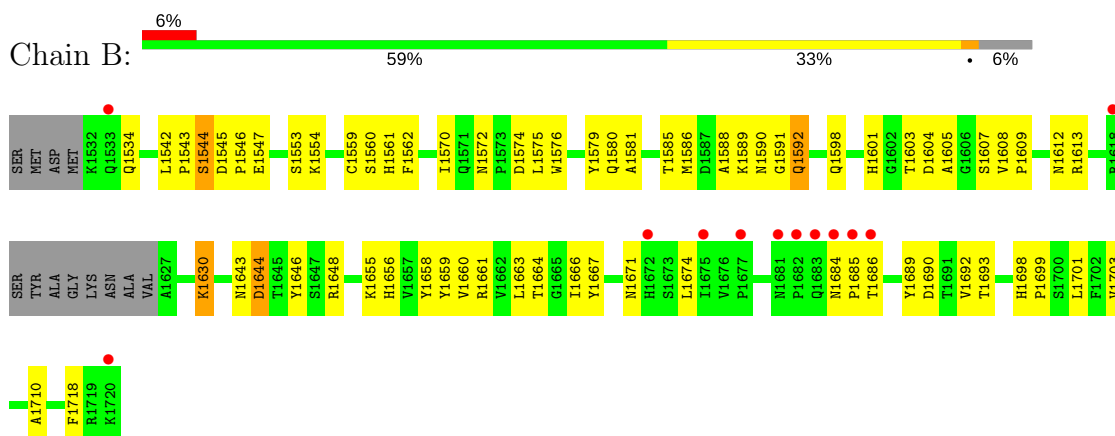
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

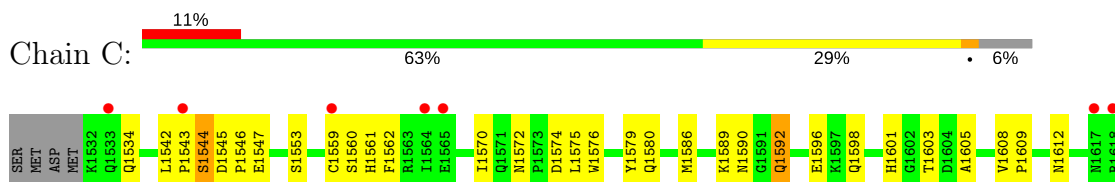
- Molecule 1: Poly [ADP-ribose] polymerase 14

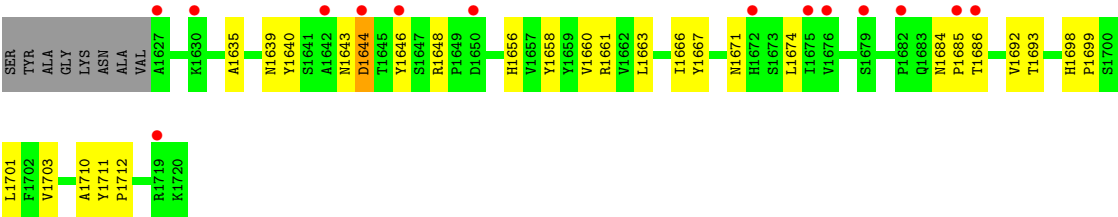


- Molecule 1: Poly [ADP-ribose] polymerase 14

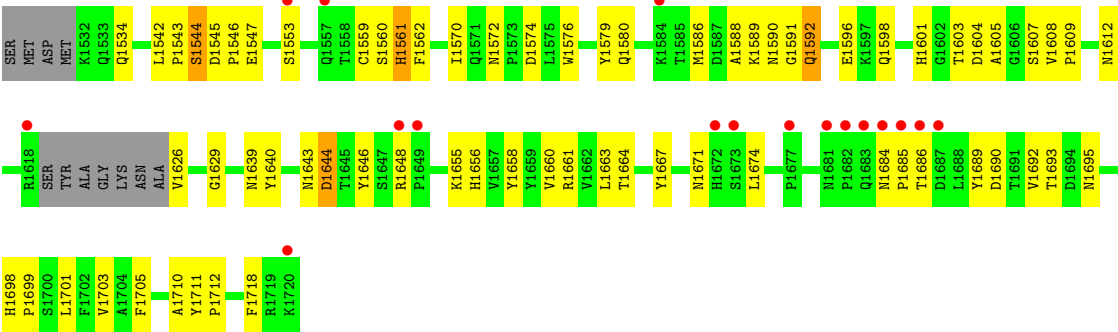


- Molecule 1: Poly [ADP-ribose] polymerase 14





● 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, $\alpha$ , $\beta$ , $\gamma$	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) 98.9 (24.56-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.253 , 0.292 0.239 , 0.289	Depositor DCC
$R_{free}$ test set	1118 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 93.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.42	0/1489	0.52	0/2028
1	B	0.41	0/1492	0.52	0/2033
1	C	0.36	0/1484	0.50	0/2024
1	D	0.38	0/1496	0.51	0/2040
All	All	0.39	0/5961	0.51	0/8125

There are no bond length outliers.

There are no bond angle outliers.

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	56	0
1	B	1450	0	1346	60	0
1	C	1442	0	1328	53	0
1	D	1454	0	1346	60	0
2	A	10	0	8	2	0
2	B	10	0	8	0	0
2	C	10	0	8	1	0
2	D	10	0	8	0	0
All	All	5834	0	5385	213	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 19.

All (213) 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: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:1551:VAL:C	1:A:1552:ALA:CA	2.53	0.76
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: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: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:1572:ASN:C	1:A:1572:ASN:OD1	2.34	0.66
1:B:1572:ASN:C	1:B:1572:ASN:OD1	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:1546:PRO:HG2	1:C:1547:GLU:H	1.74	0.53
1:C:1701:LEU:C	1:C:1701:LEU:HD12	2.29	0.53
1:D:1579:TYR:CE1	1:D:1663:LEU:HG	2.44	0.53
1:C:1543:PRO:O	1:C:1544:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1588:ALA:O	1:D:1689:TYR:OH	2.26	0.53
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: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:D:1543:PRO:O	1:D:1544:SER:HB2	2.10	0.51
1:A:1701:LEU:HD12	1:A:1701:LEU:C	2.31	0.51
1:C:1643:ASN:HB2	1:C:1646:TYR:CD2	2.45	0.51
1:D:1701:LEU:C	1:D:1701:LEU:HD12	2.31	0.51
1:A:1579:TYR:CE1	1:A:1663:LEU:HG	2.46	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:B:1572:ASN:OD1	1:B:1572:ASN:O	2.29	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:D:1560:SER:C	1:D:1562:PHE:H	2.15	0.50
1:D:1598:GLN:HA	1:D:1660:VAL:O	2.11	0.50
1:A:1572:ASN:O	1:A:1572:ASN:OD1	2.30	0.50
1:A:1534:GLN:O	1:A:1572:ASN:ND2	2.45	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:A:1560:SER:C	1:A:1562:PHE:H	2.16	0.48
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:O	1:A:1701:LEU:HD12	2.14	0.48
1:B:1701:LEU:C	1:B:1701:LEU:HD12	2.33	0.48
1:D:1576:TRP:CZ2	1:D:1580:GLN:NE2	2.80	0.48
1:C:1560:SER:C	1:C:1562:PHE:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:1701:LEU:HD12	2.14	0.47
1:B:1560:SER:C	1:B:1562:PHE:H	2.17	0.47
1:A:1684:ASN:C	1:A:1686:THR:H	2.18	0.47
1:B:1684:ASN:C	1:B:1686:THR:H	2.19	0.46
1:A:1598:GLN:HA	1:A:1660:VAL:O	2.15	0.46
1:C:1635:ALA:HB2	2:C:1:3AB:H6	1.97	0.46
1:C:1612:ASN:ND2	1:C:1658:TYR:OH	2.48	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:C:1684:ASN:C	1:C:1686:THR:H	2.19	0.46
1:D:1684:ASN:C	1:D:1686:THR:H	2.19	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:O	1:B:1701:LEU:HD12	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: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:HB3	1:B:1648:ARG:CZ	2.47	0.45
1:C:1575:LEU:HA	1:C:1575:LEU:HD23	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:1586:MET:HE1	1:D:1663:LEU:HB3	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1711:TYR:HA	1:C:1712:PRO:HD3	1.84	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: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: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:1586:MET:HE1	1:C:1663:LEU:HB3	2.01	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:H	1:D:1561:HIS:CD2	2.36	0.42
1:B:1559:CYS:O	1:B:1562:PHE:HB2	2.19	0.42
1:B:1581:ALA:O	1:B:1585:THR:HG23	2.20	0.42
1:D:1648:ARG:HB3	1:D:1648:ARG:CZ	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:D:1692:VAL:HG22	1:D:1705:PHE:HE2	1.85	0.42
1:D:1695:ASN:OD1	1:D:1695:ASN:C	2.58	0.42
1:A:1559:CYS:O	1:A:1562:PHE:HB2	2.19	0.41
1:D:1572:ASN:C	1:D:1572:ASN:OD1	2.58	0.41
1:D:1579:TYR:OH	1:D:1596:GLU:HG3	2.20	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: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:D:1701:LEU:O	1:D:1701:LEU:HD12	2.20	0.41
1:B:1664:THR:O	1:B:1690:ASP:HB2	2.20	0.41
1:B:1613:ARG:HE	1:B:1613:ARG:HB2	1.70	0.41
1:D:1698:HIS:N	1:D:1699:PRO:HD3	2.35	0.41
1:A:1579:TYR:OH	1:A:1596:GLU:HG3	2.20	0.41
1:B:1630:LYS:HB2	1:B:1630:LYS:HZ1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1592:GLN:HG3	1:B:1592:GLN:H	1.34	0.41
1:A:1667:TYR:CD1	1:C:1592:GLN:HG2	2.56	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:B:1554:LYS:HD2	1:B:1659:TYR:CZ	2.56	0.40
1:B:1590:ASN:O	1:B:1591:GLY:C	2.59	0.40
1:B:1604:ASP:OD1	1:B:1607:SER:N	2.54	0.40
1:D:1590:ASN:O	1:D:1591:GLY:C	2.59	0.40
1:D:1664:THR:O	1:D:1690:ASP:HB2	2.22	0.40
1:A:1586:MET:HE1	1:A:1663:LEU:HB3	2.02	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%)	7	25
1	B	177/193 (92%)	159 (90%)	15 (8%)	3 (2%)	11	34
1	C	177/193 (92%)	159 (90%)	15 (8%)	3 (2%)	11	34
1	D	178/193 (92%)	157 (88%)	17 (10%)	4 (2%)	8	26
All	All	707/772 (92%)	630 (89%)	63 (9%)	14 (2%)	9	28

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1544	SER
1	B	1544	SER
1	C	1544	SER

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Mol	Chain	Res	Type
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 [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	155/170 (91%)	153 (99%)	2 (1%)	73	93
1	B	156/170 (92%)	153 (98%)	3 (2%)	62	89
1	C	154/170 (91%)	152 (99%)	2 (1%)	73	93
1	D	156/170 (92%)	154 (99%)	2 (1%)	73	93
All	All	621/680 (91%)	612 (99%)	9 (1%)	71	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1592	GLN
1	A	1644	ASP
1	B	1592	GLN
1	B	1630	LYS
1	B	1644	ASP
1	C	1592	GLN
1	C	1644	ASP
1	D	1592	GLN
1	D	1644	ASP



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1534	GLN
1	A	1561	HIS
1	A	1612	ASN
1	A	1671	ASN
1	B	1534	GLN
1	B	1561	HIS
1	B	1612	ASN
1	B	1671	ASN
1	B	1683	GLN
1	C	1534	GLN
1	C	1561	HIS
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 carbohydrates 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	A	1	-	10,10,10	1.62	1 (10%)	13,13,13	1.59	3 (23%)
2	3AB	B	1	-	10,10,10	0.75	0	13,13,13	1.29	1 (7%)
2	3AB	C	1	-	10,10,10	0.75	0	13,13,13	1.16	1 (7%)
2	3AB	D	1	-	10,10,10	0.65	0	13,13,13	1.48	2 (15%)

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	A	1	-	-	0/4/4/4	0/1/1/1
2	3AB	B	1	-	-	0/4/4/4	0/1/1/1
2	3AB	C	1	-	-	0/4/4/4	0/1/1/1
2	3AB	D	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	-2.24	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'	-3.89	113.33	117.77
2	B	1	3AB	C1-C1'-N1'	-3.58	113.68	117.77
2	C	1	3AB	C1-C1'-N1'	-3.07	114.27	117.77
2	A	1	3AB	C1-C1'-N1'	-2.93	114.43	117.77
2	A	1	3AB	C1-C2-C3	-2.66	118.45	120.67
2	A	1	3AB	C6-C1-C2	2.05	121.64	119.23
2	D	1	3AB	O1'-C1'-N1'	2.21	125.72	122.58

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	181/193 (93%)	0.38	13 (7%) 16 9	61, 75, 123, 179	0
1	B	181/193 (93%)	0.21	12 (6%) 19 11	27, 63, 122, 178	0
1	C	181/193 (93%)	0.75	21 (11%) 5 3	67, 86, 130, 180	0
1	D	182/193 (94%)	0.35	17 (9%) 9 5	33, 67, 124, 179	0
All	All	725/772 (93%)	0.42	63 (8%) 11 6	27, 75, 130, 180	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1682	PRO	6.2
1	D	1618	ARG	5.9
1	C	1685	PRO	5.7
1	D	1685	PRO	5.6
1	C	1627	ALA	5.4
1	D	1684	ASN	5.3
1	A	1685	PRO	4.9
1	B	1686	THR	4.7
1	B	1683	GLN	4.6
1	C	1564	ILE	4.4
1	B	1685	PRO	4.2
1	A	1686	THR	3.9
1	C	1675	ILE	3.8
1	B	1681	ASN	3.7
1	A	1672	HIS	3.6
1	D	1683	GLN	3.6
1	A	1681	ASN	3.6
1	D	1720	LYS	3.5
1	A	1683	GLN	3.5
1	D	1682	PRO	3.5
1	C	1618	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	1557	GLN	3.3
1	C	1686	THR	3.2
1	C	1533	GLN	3.2
1	D	1681	ASN	3.2
1	B	1675	ILE	3.1
1	B	1684	ASN	3.1
1	D	1672	HIS	3.1
1	C	1617	ASN	2.9
1	D	1687	ASP	2.9
1	B	1533	GLN	2.9
1	C	1672	HIS	2.9
1	C	1682	PRO	2.9
1	C	1565	GLU	2.9
1	D	1686	THR	2.6
1	C	1644	ASP	2.6
1	C	1679	SER	2.6
1	B	1720	LYS	2.6
1	C	1642	ALA	2.6
1	D	1673	SER	2.6
1	A	1673	SER	2.6
1	A	1697	HIS	2.5
1	C	1559	CYS	2.5
1	D	1649	PRO	2.5
1	C	1646	TYR	2.4
1	A	1627	ALA	2.4
1	C	1630	LYS	2.4
1	C	1650	ASP	2.4
1	A	1533	GLN	2.4
1	A	1684	ASN	2.4
1	B	1672	HIS	2.3
1	C	1543	PRO	2.3
1	B	1682	PRO	2.3
1	A	1585	THR	2.3
1	D	1553	SER	2.3
1	A	1532	LYS	2.3
1	C	1676	VAL	2.3
1	D	1584	LYS	2.2
1	D	1648	ARG	2.2
1	B	1677	PRO	2.1
1	C	1719	ARG	2.1
1	B	1618	ARG	2.0
1	D	1677	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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	3AB	D	1	10/10	0.93	0.24	2.10	39,58,80,85	0
2	3AB	B	1	10/10	0.94	0.21	0.34	17,47,83,93	0
2	3AB	A	1	10/10	0.94	0.17	-0.33	10,25,49,63	0
2	3AB	C	1	10/10	0.87	0.18	-0.55	48,74,88,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.