



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:57 PM GMT

PDB ID : 4NA0  
Title : Crystal structure of mouse poly(ADP-ribose) glycohydrolase (PARG) catalytic domain with ADPRibose  
Authors : Wang, Z.; Cheng, Z.; Xu, W.  
Deposited on : 2013-10-21  
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](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 (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

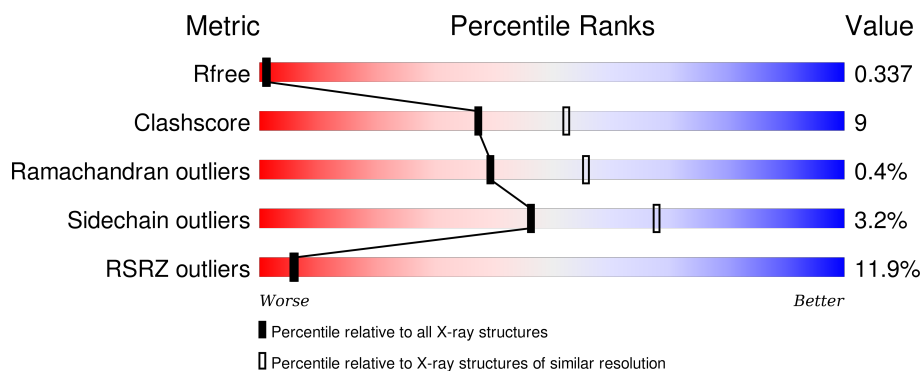
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 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	522	
1	B	522	
1	C	522	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12337 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) glycohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	Se	0	0	0
			4074	2603	710	738	14	9			
1	B	502	Total	C	N	O	S	Se	0	0	0
			4079	2605	710	741	14	9			
1	C	501	Total	C	N	O	S	Se	0	0	0
			4070	2598	709	741	13	9			

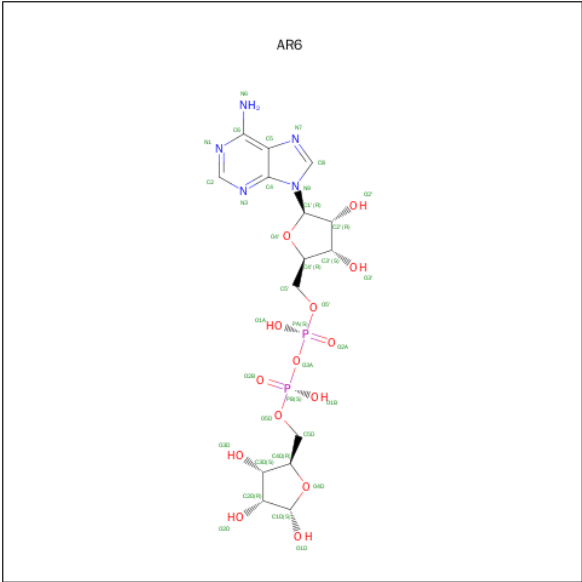
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	GLY	-	EXPRESSION TAG	UNP O88622
B	438	GLY	-	EXPRESSION TAG	UNP O88622
C	438	GLY	-	EXPRESSION TAG	UNP O88622

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total I 2 2	0	0
2	A	2	Total I 2 2	0	0
2	C	2	Total I 2 2	0	0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).

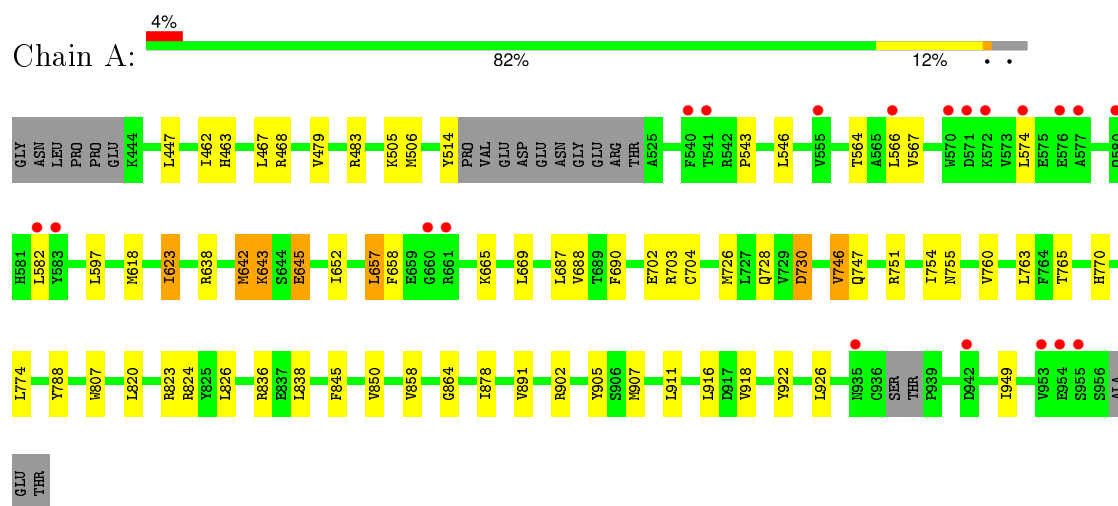


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

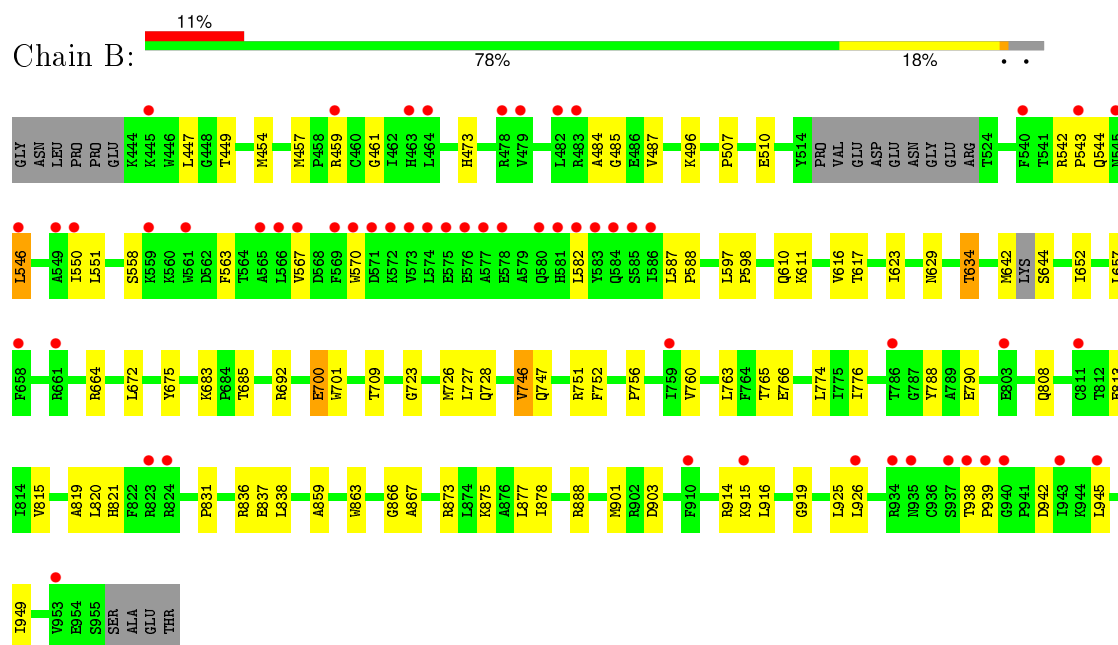
### 3 Residue-property plots

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.

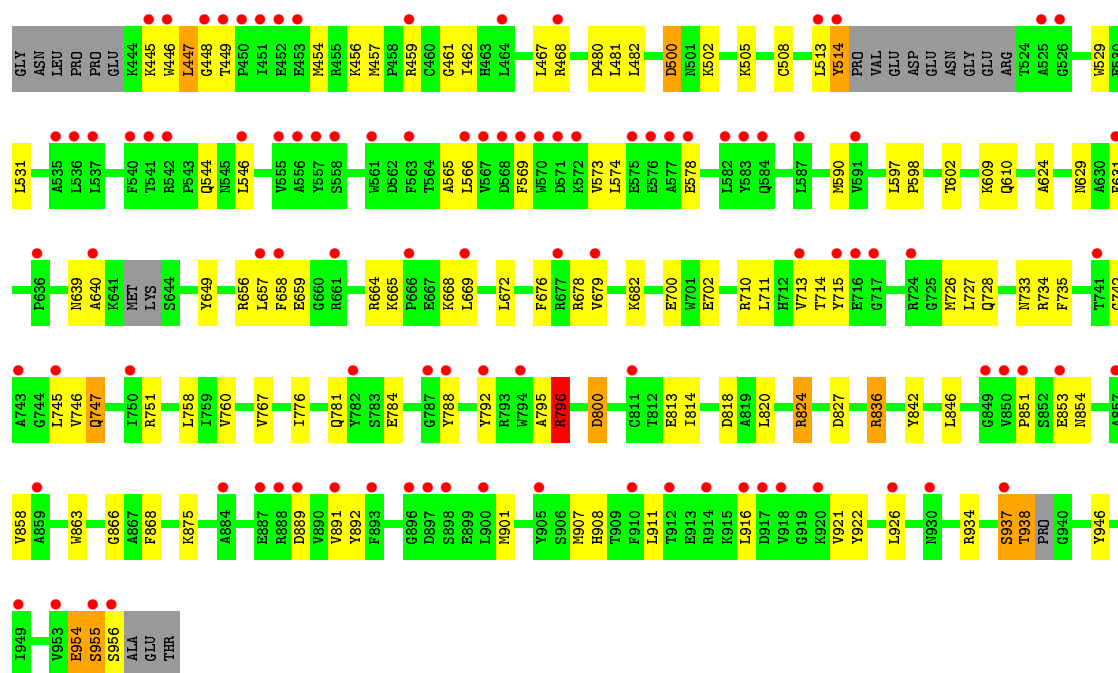
- Molecule 1: Poly(ADP-ribose) glycohydrolase



- Molecule 1: Poly(ADP-ribose) glycohydrolase



- Molecule 1: Poly(ADP-ribose) glycohydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.30Å 55.66Å 166.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 47.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.40) 97.6 (47.74-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.298 , 0.342 0.294 , 0.337	Depositor DCC
$R_{free}$ test set	3419 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	12 of 67616 reflections (0.018%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	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 70.75 % 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 2.9603e-06. 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, 0.375 respectively for untwinned datasets, and 0.333, 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: IOD, AR6

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	0.36	0/4165	0.55	0/5617
1	B	0.37	0/4170	0.53	0/5627
1	C	0.38	0/4159	0.55	1/5610 (0.0%)
All	All	0.37	0/12494	0.54	1/16854 (0.0%)

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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	796	ARG	NE-CZ-NH1	6.19	123.39	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	700	GLU	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	4074	0	4042	59	0
1	B	4079	0	4042	66	0
1	C	4070	0	4030	103	0
2	A	2	0	0	2	0
2	B	2	0	0	0	0
2	C	2	0	0	1	0
3	A	36	0	20	2	0
3	B	36	0	20	2	0
3	C	36	0	21	6	0
All	All	12337	0	12175	229	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 9.

All (229) 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:A:907:MSE:HE1	1:A:949:ILE:HG21	1.22	1.09
1:C:447:LEU:CD2	1:C:713:VAL:HG23	1.86	1.05
1:B:726:MSE:HE3	1:B:859:ALA:HB2	1.39	1.04
1:C:711:LEU:HD21	1:C:713:VAL:HG13	1.41	1.00
1:A:618:MSE:HE3	1:A:623:ILE:CD1	1.94	0.98
1:A:907:MSE:HE3	1:A:911:LEU:HD11	1.49	0.93
1:C:713:VAL:HG12	1:C:892:TYR:HB3	1.51	0.92
1:C:447:LEU:HD23	1:C:713:VAL:HG23	1.54	0.90
1:C:447:LEU:HD22	1:C:447:LEU:N	1.87	0.90
1:C:447:LEU:HD21	1:C:713:VAL:HG23	1.52	0.89
1:C:911:LEU:HD21	1:C:921:VAL:HG22	1.55	0.88
1:B:447:LEU:HG	1:B:901:MSE:HE3	1.57	0.86
1:C:447:LEU:HD23	1:C:713:VAL:CG2	2.07	0.85
1:B:728:GLN:OE1	1:B:751:ARG:NH2	2.14	0.81
1:A:728:GLN:OE1	1:A:751:ARG:NH2	2.14	0.81
1:A:907:MSE:HE1	1:A:949:ILE:CG2	2.09	0.79
1:B:447:LEU:HG	1:B:901:MSE:CE	2.11	0.79
1:C:711:LEU:HD21	1:C:713:VAL:CG1	2.12	0.78
1:C:858:VAL:HG12	1:C:889:ASP:O	1.84	0.78
1:A:467:LEU:O	1:A:479:VAL:HG11	1.83	0.78
1:A:907:MSE:CE	1:A:949:ILE:HG21	2.11	0.77
1:B:726:MSE:CE	1:B:859:ALA:HB2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:LEU:N	1:C:447:LEU:CD2	2.51	0.73
1:C:624:ALA:HB1	1:C:679:VAL:HG11	1.69	0.73
1:C:711:LEU:CD2	1:C:713:VAL:HG13	2.18	0.72
1:B:629:ASN:OD1	1:B:634:THR:HG21	1.90	0.72
1:C:447:LEU:HD21	1:C:901:MSE:HG2	1.73	0.71
1:C:514:TYR:CE2	1:C:531:LEU:HD22	2.26	0.71
1:C:746:VAL:HG13	1:C:788:TYR:OH	1.90	0.71
1:B:723:GLY:HA2	1:B:726:MSE:HE2	1.73	0.70
1:C:447:LEU:CD2	1:C:713:VAL:CG2	2.65	0.70
1:A:618:MSE:CE	1:A:623:ILE:CD1	2.70	0.70
1:A:746:VAL:HG13	1:A:747:GLN:H	1.56	0.70
1:B:746:VAL:HG22	1:B:788:TYR:OH	1.90	0.69
1:B:709:THR:HG21	1:B:888:ARG:O	1.91	0.69
1:A:618:MSE:HE3	1:A:623:ILE:HD13	1.72	0.69
1:B:692:ARG:NH2	1:B:766:GLU:O	2.26	0.68
1:A:820:LEU:HD11	1:A:836:ARG:HG2	1.76	0.67
1:C:746:VAL:HG11	3:C:1003:AR6:O2A	1.96	0.65
1:C:665:LYS:O	1:C:669:LEU:HD23	1.97	0.65
1:C:818:ASP:O	1:C:836:ARG:NH2	2.30	0.64
1:A:618:MSE:HE3	1:A:623:ILE:HD11	1.77	0.64
1:A:623:ILE:HD11	1:A:688:VAL:HG21	1.80	0.63
1:A:746:VAL:HG13	1:A:747:GLN:N	2.14	0.63
1:A:907:MSE:HE3	1:A:911:LEU:CD1	2.26	0.62
1:C:447:LEU:HD21	1:C:901:MSE:CG	2.29	0.62
1:B:746:VAL:HG13	1:B:747:GLN:N	2.14	0.62
1:C:781:GLN:N	1:C:800:ASP:OD2	2.32	0.62
1:C:715:TYR:H	1:C:901:MSE:HE2	1.63	0.62
1:B:657:LEU:HD21	1:B:672:LEU:HD12	1.81	0.62
1:B:838:LEU:HD23	1:B:878:ILE:HG23	1.82	0.62
1:C:824:ARG:HB3	1:C:827:ASP:HB2	1.82	0.61
1:C:668:LYS:NZ	1:C:742:GLY:O	2.34	0.61
1:A:618:MSE:CE	1:A:623:ILE:HD11	2.31	0.60
1:B:597:LEU:HD22	1:B:629:ASN:ND2	2.16	0.60
1:A:514:TYR:C	2:A:1002:IOD:I	3.10	0.60
1:A:687:LEU:HD12	1:A:807:TRP:O	2.00	0.60
1:A:618:MSE:HE2	1:A:690:PHE:CE1	2.37	0.59
1:A:704:CYS:HB3	1:A:918:VAL:HG23	1.83	0.59
1:C:715:TYR:N	1:C:901:MSE:HE2	2.18	0.59
1:A:657:LEU:HD12	1:A:669:LEU:HD21	1.85	0.59
1:C:784:GLU:O	1:C:795:ALA:HB3	2.01	0.59
1:B:487:VAL:HG21	1:B:683:LYS:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:MSE:HE3	1:A:623:ILE:CG1	2.33	0.58
1:C:858:VAL:CG1	1:C:889:ASP:O	2.51	0.58
1:C:911:LEU:HD21	1:C:921:VAL:CG2	2.30	0.58
1:A:746:VAL:HG22	1:A:788:TYR:OH	2.04	0.58
1:C:566:LEU:HD13	1:C:658:PHE:CD1	2.39	0.57
1:A:447:LEU:HD13	1:A:905:TYR:CD2	2.40	0.57
1:A:462:ILE:HD11	1:A:850:VAL:HG13	1.86	0.57
1:C:457:MSE:SE	1:C:461:GLY:HA2	2.54	0.57
1:B:867:ALA:HB3	3:B:1003:AR6:O5D	2.05	0.57
1:B:727:LEU:HD13	1:B:813:GLU:OE2	2.05	0.57
1:C:590:MSE:HE1	1:C:631:PHE:CG	2.40	0.56
1:B:746:VAL:HG13	1:B:747:GLN:H	1.69	0.56
1:C:624:ALA:CB	1:C:679:VAL:HG11	2.35	0.56
1:A:657:LEU:HD12	1:A:669:LEU:CD2	2.35	0.56
1:B:863:TRP:O	1:B:875:LYS:HG2	2.06	0.55
1:B:837:GLU:OE2	1:B:875:LYS:NZ	2.25	0.55
1:C:480:ASP:OD2	1:C:481:LEU:HD12	2.06	0.55
1:A:642:MET:HG2	1:A:643:LYS:N	2.22	0.55
1:A:638:ARG:NH2	1:A:763:LEU:O	2.39	0.55
1:C:598:PRO:O	1:C:602:THR:HG22	2.06	0.55
1:C:446:TRP:C	1:C:447:LEU:HD22	2.28	0.55
1:A:765:THR:HG21	1:A:774:LEU:HD22	1.89	0.55
1:C:863:TRP:O	1:C:875:LYS:HG2	2.07	0.54
1:C:937:SER:O	1:C:938:THR:HG23	2.07	0.54
1:C:851:PRO:HB2	1:C:854:ASN:HD22	1.72	0.54
1:A:746:VAL:HG13	3:A:1003:AR6:O2A	2.08	0.54
1:B:616:VAL:HG13	1:B:616:VAL:O	2.08	0.54
1:C:569:PHE:CE2	1:C:574:LEU:HD11	2.43	0.54
1:B:664:ARG:NH1	1:B:790:GLU:O	2.41	0.54
1:B:820:LEU:HD11	1:B:836:ARG:HD2	1.88	0.54
1:A:623:ILE:HD13	1:A:760:VAL:HG11	1.90	0.54
1:A:726:MSE:SE	1:A:891:VAL:HG21	2.58	0.54
1:C:728:GLN:OE1	1:C:751:ARG:NH2	2.40	0.54
1:C:911:LEU:HD11	1:C:916:LEU:HD23	1.90	0.54
1:C:820:LEU:HD11	1:C:836:ARG:HG2	1.90	0.54
1:B:657:LEU:HD21	1:B:672:LEU:CD1	2.37	0.54
1:B:485:GLY:O	1:B:685:THR:HG21	2.08	0.54
1:A:826:LEU:HD23	1:A:826:LEU:O	2.08	0.53
1:A:618:MSE:HE3	1:A:623:ILE:HG12	1.91	0.53
1:C:639:ASN:O	1:C:640:ALA:HB2	2.09	0.53
1:B:914:ARG:O	1:B:915:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:GLU:O	1:C:955:SER:C	2.46	0.53
1:C:513:LEU:O	1:C:514:TYR:CD2	2.62	0.52
1:C:866:GLY:HA3	3:C:1003:AR6:O1A	2.09	0.52
1:A:618:MSE:HE2	1:A:690:PHE:HE1	1.73	0.52
1:A:911:LEU:HD22	1:A:916:LEU:HD12	1.91	0.52
1:C:456:LYS:CE	1:C:726:MSE:HE2	2.40	0.52
1:A:704:CYS:SG	1:A:918:VAL:HG21	2.50	0.51
1:A:746:VAL:CG1	1:A:747:GLN:N	2.74	0.51
1:B:642:MET:O	1:B:644:SER:N	2.44	0.51
1:C:665:LYS:HE2	2:C:1001:IOD:I	2.81	0.51
1:B:507:PRO:CB	1:B:634:THR:HG23	2.41	0.50
1:B:551:LEU:HD22	1:B:558:SER:HA	1.93	0.50
1:C:784:GLU:HB3	1:C:796:ARG:HD3	1.93	0.50
1:A:564:THR:O	1:A:567:VAL:HG22	2.12	0.50
1:C:746:VAL:CG1	1:C:747:GLN:N	2.75	0.50
1:B:831:PRO:HG3	1:B:926:LEU:HD13	1.93	0.50
1:B:507:PRO:HB3	1:B:634:THR:HG23	1.94	0.50
1:C:500:ASP:O	1:C:505:LYS:NZ	2.44	0.50
1:C:449:THR:HG21	1:C:710:ARG:NE	2.27	0.49
1:C:454:MSE:HE1	1:C:889:ASP:HB3	1.93	0.49
1:A:754:ILE:HG13	1:A:755:ASN:HD22	1.78	0.49
1:A:566:LEU:HD13	1:A:658:PHE:CD1	2.46	0.49
1:A:543:PRO:HB2	1:A:567:VAL:HG12	1.94	0.49
1:C:610:GLN:HE21	1:C:767:VAL:HG13	1.78	0.49
1:B:652:ILE:HG12	1:B:763:LEU:HD13	1.93	0.49
1:C:922:TYR:CE2	1:C:926:LEU:HD11	2.48	0.49
1:C:746:VAL:HG12	1:C:747:GLN:N	2.28	0.49
1:C:866:GLY:HA3	3:C:1003:AR6:O3'	2.11	0.49
1:C:678:ARG:NH1	1:C:682:LYS:O	2.46	0.49
1:B:449:THR:HB	1:B:454:MSE:HE2	1.94	0.49
1:A:618:MSE:CE	1:A:623:ILE:HD13	2.38	0.49
1:C:462:ILE:HD12	1:C:462:ILE:C	2.33	0.49
3:C:1003:AR6:C3'	3:C:1003:AR6:O1A	2.60	0.48
1:B:938:THR:HG23	1:B:939:PRO:HD2	1.96	0.48
1:B:587:LEU:HB2	1:B:588:PRO:HD3	1.95	0.48
1:C:447:LEU:HD23	1:C:713:VAL:HG22	1.90	0.48
1:B:752:PHE:O	1:B:756:PRO:HA	2.13	0.48
1:B:473:HIS:NE2	1:B:617:THR:OG1	2.36	0.48
1:B:507:PRO:HG3	1:B:634:THR:CG2	2.44	0.48
1:A:746:VAL:HG22	1:A:788:TYR:CZ	2.49	0.47
1:A:574:LEU:CD1	1:A:582:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:GLU:H	1:B:700:GLU:CD	2.16	0.47
1:C:733:ASN:HD22	1:C:735:PHE:H	1.61	0.47
1:C:514:TYR:CZ	1:C:531:LEU:HD22	2.49	0.47
1:B:746:VAL:HG22	1:B:788:TYR:CZ	2.50	0.47
1:A:652:ILE:HG12	1:A:763:LEU:HD13	1.95	0.47
1:A:462:ILE:HG22	1:A:463:HIS:N	2.30	0.47
1:C:657:LEU:HD11	1:C:672:LEU:CD1	2.45	0.47
1:A:845:PHE:CE1	1:A:858:VAL:HG11	2.50	0.46
1:A:907:MSE:HE2	1:A:949:ILE:HD13	1.96	0.46
1:C:573:VAL:HG12	1:C:573:VAL:O	2.15	0.46
1:B:866:GLY:HA3	3:B:1003:AR6:O5'	2.16	0.46
1:C:776:ILE:HD12	1:C:776:ILE:N	2.29	0.46
1:A:864:GLY:HA2	3:A:1003:AR6:O2B	2.15	0.46
1:C:597:LEU:HD22	1:C:629:ASN:ND2	2.30	0.46
1:B:484:ALA:HB2	1:B:808:GLN:HE22	1.81	0.46
1:B:945:LEU:HD11	1:B:949:ILE:HD11	1.98	0.46
1:C:842:TYR:CZ	1:C:846:LEU:HD22	2.50	0.46
1:C:447:LEU:HD21	1:C:901:MSE:SE	2.66	0.46
1:C:454:MSE:HE2	1:C:891:VAL:HG23	1.97	0.46
1:B:675:TYR:CG	1:B:756:PRO:HG2	2.51	0.46
1:C:784:GLU:HB3	1:C:796:ARG:CD	2.45	0.45
1:C:597:LEU:N	1:C:598:PRO:HD2	2.32	0.45
1:A:770:HIS:CD2	1:A:836:ARG:HE	2.35	0.45
1:A:704:CYS:SG	1:A:918:VAL:CG2	3.04	0.45
1:B:727:LEU:HD11	1:B:815:VAL:CG1	2.46	0.45
1:C:456:LYS:HE2	1:C:726:MSE:HE2	1.97	0.45
1:C:467:LEU:HD12	1:C:468:ARG:N	2.32	0.45
1:B:542:ARG:HB2	1:B:543:PRO:HD2	1.99	0.45
1:C:668:LYS:HE3	1:C:745:LEU:HG	1.99	0.44
1:C:745:LEU:HD22	1:C:792:TYR:CG	2.52	0.44
1:A:665:LYS:HD2	2:A:1001:IOD:I	2.87	0.44
1:A:506:MSE:HE1	1:A:597:LEU:HD11	1.99	0.44
1:C:565:ALA:HB3	1:C:658:PHE:O	2.18	0.44
1:B:610:GLN:O	1:B:611:LYS:HB2	2.17	0.44
1:B:873:ARG:NH2	1:B:903:ASP:OD2	2.47	0.44
1:C:590:MSE:HE3	1:C:676:PHE:CD1	2.53	0.44
1:B:776:ILE:HD12	1:B:776:ILE:N	2.32	0.44
1:C:796:ARG:HG2	1:C:796:ARG:HH11	1.82	0.44
1:C:796:ARG:CG	1:C:796:ARG:HH11	2.30	0.44
1:C:727:LEU:HD13	1:C:813:GLU:HG2	2.00	0.43
1:C:569:PHE:CZ	1:C:574:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:819:ALA:HB2	1:B:863:TRP:CE2	2.52	0.43
1:B:701:TRP:O	1:B:919:GLY:HA2	2.17	0.43
1:C:656:ARG:NE	1:C:659:GLU:OE1	2.42	0.43
1:C:955:SER:O	1:C:956:SER:CB	2.67	0.43
1:C:508:CYS:HA	1:C:529:TRP:CD2	2.54	0.43
1:C:449:THR:HG21	1:C:710:ARG:CZ	2.49	0.43
1:C:574:LEU:HD22	1:C:578:GLU:HB3	2.01	0.43
1:C:500:ASP:HB3	1:C:502:LYS:H	1.83	0.43
1:A:730:ASP:OD2	1:A:730:ASP:C	2.56	0.43
1:B:838:LEU:CD2	1:B:878:ILE:HG23	2.48	0.42
1:C:911:LEU:CD1	1:C:916:LEU:HD23	2.49	0.42
1:B:597:LEU:N	1:B:598:PRO:HD2	2.35	0.42
1:C:758:LEU:HD11	1:C:814:ILE:HD12	2.01	0.42
1:C:609:LYS:HG2	1:C:649:TYR:OH	2.19	0.42
1:A:838:LEU:HD23	1:A:878:ILE:HG23	2.02	0.42
1:B:820:LEU:CD1	1:B:836:ARG:HD2	2.50	0.42
1:B:543:PRO:HG3	1:B:570:TRP:HB3	2.02	0.42
1:C:746:VAL:CG1	3:C:1003:AR6:O2A	2.65	0.42
1:B:563:PHE:O	1:B:567:VAL:HG23	2.19	0.42
1:C:711:LEU:C	1:C:711:LEU:HD23	2.40	0.42
1:B:726:MSE:HE3	1:B:859:ALA:CB	2.29	0.42
1:C:454:MSE:HE1	1:C:889:ASP:CB	2.50	0.42
1:C:456:LYS:NZ	1:C:726:MSE:HE2	2.35	0.42
1:C:868:PHE:CD1	3:C:1003:AR6:H5DA	2.55	0.41
1:A:922:TYR:CZ	1:A:926:LEU:HD11	2.55	0.41
1:C:454:MSE:HE2	1:C:891:VAL:CG2	2.50	0.41
1:A:483:ARG:HA	1:A:483:ARG:NE	2.35	0.41
1:B:546:LEU:HD22	1:B:550:ILE:CD1	2.51	0.41
1:A:505:LYS:NZ	1:A:645:GLU:OE1	2.52	0.41
1:B:457:MSE:SE	1:B:461:GLY:CA	3.18	0.41
1:C:746:VAL:O	1:C:747:GLN:C	2.58	0.41
1:B:765:THR:HG21	1:B:774:LEU:HD22	2.02	0.41
1:B:877:LEU:HD23	1:B:925:LEU:HD21	2.03	0.41
1:B:623:ILE:HG12	1:B:760:VAL:HG11	2.01	0.41
1:C:907:MSE:HE3	1:C:946:TYR:HA	2.02	0.41
1:C:448:GLY:HA3	1:C:711:LEU:O	2.21	0.41
1:C:711:LEU:HD13	1:C:908:HIS:ND1	2.36	0.41
1:C:454:MSE:CE	1:C:891:VAL:HG23	2.51	0.41
1:B:746:VAL:CG1	1:B:747:GLN:N	2.83	0.41
1:C:590:MSE:HE3	1:C:676:PHE:CE1	2.56	0.40
1:B:727:LEU:HD11	1:B:815:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:914:ARG:O	1:B:916:LEU:HD12	2.21	0.40
1:B:831:PRO:CG	1:B:926:LEU:HD13	2.51	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	495/522 (95%)	473 (96%)	20 (4%)	2 (0%)	39	56
1	B	496/522 (95%)	482 (97%)	14 (3%)	0	100	100
1	C	493/522 (94%)	464 (94%)	25 (5%)	4 (1%)	24	35
All	All	1484/1566 (95%)	1419 (96%)	59 (4%)	6 (0%)	39	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	LYS
1	C	937	SER
1	C	954	GLU
1	C	747	GLN
1	C	955	SER
1	A	645	GLU

### 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	441/450 (98%)	429 (97%)	12 (3%)	52	73
1	B	442/450 (98%)	431 (98%)	11 (2%)	55	76
1	C	441/450 (98%)	421 (96%)	20 (4%)	34	52
All	All	1324/1350 (98%)	1281 (97%)	43 (3%)	46	68

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	ARG
1	A	546	LEU
1	A	623	ILE
1	A	642	MET
1	A	657	LEU
1	A	702	GLU
1	A	703	ARG
1	A	730	ASP
1	A	746	VAL
1	A	823	ARG
1	A	824	ARG
1	A	902	ARG
1	B	459	ARG
1	B	496	LYS
1	B	510	GLU
1	B	544	GLN
1	B	546	LEU
1	B	582	LEU
1	B	634	THR
1	B	700	GLU
1	B	746	VAL
1	B	821	HIS
1	B	942	ASP
1	C	445	LYS
1	C	447	LEU
1	C	459	ARG
1	C	482	LEU
1	C	500	ASP
1	C	514	TYR
1	C	544	GLN
1	C	546	LEU
1	C	664	ARG
1	C	702	GLU
1	C	714	THR

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Mol	Chain	Res	Type
1	C	734	ARG
1	C	760	VAL
1	C	796	ARG
1	C	800	ASP
1	C	824	ARG
1	C	836	ARG
1	C	853	GLU
1	C	934	ARG
1	C	938	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	544	GLN
1	A	545	ASN
1	A	755	ASN
1	A	770	HIS
1	B	545	ASN
1	B	614	HIS
1	B	770	HIS
1	C	544	GLN
1	C	610	GLN
1	C	629	ASN
1	C	733	ASN
1	C	808	GLN
1	C	854	ASN
1	C	879	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 ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AR6	A	1003	-	32,39,39	1.47	6 (18%)	39,60,60	2.50	8 (20%)
3	AR6	B	1003	-	32,39,39	1.48	5 (15%)	39,60,60	2.70	9 (23%)
3	AR6	C	1003	-	32,39,39	1.57	4 (12%)	39,60,60	2.91	10 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AR6	A	1003	-	-	0/18/54/54	0/4/4/4
3	AR6	B	1003	-	-	0/18/54/54	0/4/4/4
3	AR6	C	1003	-	-	0/18/54/54	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	AR6	O4'-C1'	2.12	1.43	1.41
3	A	1003	AR6	C2-N3	2.14	1.36	1.32
3	B	1003	AR6	O4'-C1'	2.29	1.44	1.41
3	A	1003	AR6	PA-O5'	2.50	1.70	1.59
3	B	1003	AR6	PA-O5'	2.60	1.70	1.59
3	A	1003	AR6	PA-O1A	2.80	1.66	1.54
3	C	1003	AR6	PA-O1A	2.82	1.67	1.54
3	C	1003	AR6	O4'-C1'	2.83	1.44	1.41
3	B	1003	AR6	PA-O1A	3.02	1.67	1.54
3	A	1003	AR6	PA-O2A	3.85	1.65	1.51
3	B	1003	AR6	PA-O2A	4.14	1.66	1.51
3	C	1003	AR6	PA-O2A	4.47	1.67	1.51
3	A	1003	AR6	C6-N6	4.49	1.48	1.34
3	B	1003	AR6	C6-N6	4.63	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	AR6	C6-N6	5.22	1.51	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	AR6	N3-C2-N1	-9.81	121.38	128.89
3	B	1003	AR6	N3-C2-N1	-9.72	121.45	128.89
3	A	1003	AR6	N3-C2-N1	-9.30	121.78	128.89
3	B	1003	AR6	O5'-C5'-C4'	-5.42	89.14	109.12
3	B	1003	AR6	PB-O3A-PA	-4.89	119.01	132.73
3	C	1003	AR6	PB-O3A-PA	-4.53	120.01	132.73
3	B	1003	AR6	O1A-PA-O5'	-4.41	86.25	108.46
3	A	1003	AR6	O5'-C5'-C4'	-4.30	93.25	109.12
3	C	1003	AR6	O1A-PA-O2A	-4.18	89.89	112.53
3	A	1003	AR6	O1A-PA-O5'	-4.10	87.79	108.46
3	C	1003	AR6	O5'-PA-O2A	-4.03	93.99	109.62
3	A	1003	AR6	PB-O3A-PA	-3.94	121.67	132.73
3	B	1003	AR6	C4-C5-N7	-2.68	107.01	109.48
3	B	1003	AR6	O1D-C1D-O4D	-2.60	107.81	111.22
3	C	1003	AR6	C1'-N9-C4	-2.44	123.25	126.94
3	C	1003	AR6	C4-C5-N7	-2.32	107.34	109.48
3	A	1003	AR6	C4-C5-N7	-2.14	107.51	109.48
3	C	1003	AR6	O4'-C1'-N9	2.33	112.97	108.10
3	C	1003	AR6	O3A-PB-O5D	3.11	111.19	102.94
3	B	1003	AR6	C4'-O4'-C1'	3.13	113.16	109.72
3	A	1003	AR6	C4'-O4'-C1'	3.23	113.27	109.72
3	A	1003	AR6	O5'-PA-O2A	3.50	123.20	109.62
3	B	1003	AR6	O5'-PA-O2A	4.10	125.55	109.62
3	C	1003	AR6	O1A-PA-O5'	5.74	137.43	108.46
3	A	1003	AR6	O3A-PA-O5'	7.32	122.36	102.94
3	B	1003	AR6	O3A-PA-O5'	7.45	122.70	102.94
3	C	1003	AR6	O5'-C5'-C4'	9.44	143.91	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	AR6	2	0
3	B	1003	AR6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1003	AR6	6	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	492/522 (94%)	0.31	20 (4%) 41 42	24, 56, 106, 174	0
1	B	493/522 (94%)	0.59	56 (11%) 7 7	24, 61, 130, 194	0
1	C	492/522 (94%)	1.05	100 (20%) 1 1	20, 73, 159, 254	0
All	All	1477/1566 (94%)	0.65	176 (11%) 6 6	20, 62, 136, 254	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	916	LEU	8.1
1	C	525	ALA	8.1
1	C	582	LEU	7.9
1	C	658	PHE	7.7
1	C	918	VAL	7.7
1	C	540	PHE	7.0
1	B	566	LEU	6.9
1	B	570	TRP	6.8
1	B	546	LEU	6.7
1	B	574	LEU	6.6
1	B	575	GLU	6.3
1	C	571	ASP	6.1
1	B	582	LEU	5.9
1	C	953	VAL	5.8
1	A	582	LEU	5.8
1	C	587	LEU	5.8
1	A	570	TRP	5.7
1	C	584	GLN	5.4
1	C	563	PHE	5.4
1	B	811	CYS	5.2
1	B	940	GLY	5.0
1	B	580	GLN	4.9
1	A	574	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	811	CYS	4.8
1	B	803	GLU	4.7
1	B	937	SER	4.7
1	A	580	GLN	4.7
1	C	792	TYR	4.6
1	C	661	ARG	4.6
1	B	935	ASN	4.6
1	C	570	TRP	4.5
1	C	857	ALA	4.3
1	C	575	GLU	4.2
1	C	567	VAL	4.2
1	C	577	ALA	4.1
1	C	884	ALA	4.1
1	A	571	ASP	4.1
1	C	446	TRP	4.0
1	C	782	TYR	3.9
1	C	956	SER	3.9
1	C	949	ILE	3.8
1	B	581	HIS	3.8
1	B	583	TYR	3.8
1	A	954	GLU	3.8
1	C	450	PRO	3.7
1	A	540	PHE	3.7
1	A	576	GLU	3.7
1	C	513	LEU	3.6
1	B	577	ALA	3.6
1	A	572	LYS	3.5
1	B	934	ARG	3.4
1	A	935	ASN	3.4
1	B	943	ILE	3.3
1	C	568	ASP	3.2
1	C	717	GLY	3.2
1	C	741	THR	3.2
1	C	631	PHE	3.2
1	C	572	LYS	3.2
1	C	910	PHE	3.2
1	C	905	TYR	3.2
1	C	464	LEU	3.2
1	C	889	ASP	3.2
1	C	526	GLY	3.2
1	C	578	GLU	3.1
1	A	541	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	578	GLU	3.1
1	B	464	LEU	3.1
1	B	824	ARG	3.1
1	C	576	GLU	3.1
1	C	920	LYS	3.0
1	B	483	ARG	3.0
1	C	452	GLU	3.0
1	C	679	VAL	3.0
1	C	794	TRP	3.0
1	C	888	ARG	3.0
1	B	463	HIS	3.0
1	C	851	PRO	3.0
1	A	953	VAL	2.9
1	C	541	THR	2.9
1	C	514	TYR	2.9
1	C	448	GLY	2.9
1	A	955	SER	2.9
1	C	955	SER	2.9
1	B	910	PHE	2.9
1	B	573	VAL	2.8
1	C	745	LEU	2.8
1	B	565	ALA	2.8
1	C	451	ILE	2.8
1	B	540	PHE	2.8
1	B	545	ASN	2.8
1	B	445	LYS	2.8
1	B	569	PHE	2.7
1	C	849	GLY	2.7
1	C	914	ARG	2.7
1	C	912	THR	2.7
1	B	915	LYS	2.7
1	C	557	TYR	2.7
1	B	459	ARG	2.7
1	A	583	TYR	2.7
1	C	449	THR	2.6
1	B	572	LYS	2.6
1	C	900	LEU	2.6
1	C	716	GLU	2.6
1	B	926	LEU	2.6
1	C	787	GLY	2.6
1	C	556	ALA	2.6
1	C	468	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	759	ILE	2.5
1	B	938	THR	2.5
1	B	661	ARG	2.5
1	C	891	VAL	2.5
1	C	893	PHE	2.5
1	C	536	LEU	2.5
1	C	853	GLU	2.5
1	C	750	ILE	2.5
1	B	584	GLN	2.5
1	C	897	ASP	2.5
1	C	591	VAL	2.5
1	C	537	LEU	2.5
1	B	586	ILE	2.5
1	C	715	TYR	2.5
1	C	788	TYR	2.4
1	C	636	PRO	2.4
1	B	559	LYS	2.4
1	C	561	TRP	2.4
1	C	724	ARG	2.4
1	C	859	ALA	2.4
1	B	939	PRO	2.4
1	C	666	PRO	2.4
1	B	550	ILE	2.4
1	C	930	ASN	2.4
1	C	569	PHE	2.4
1	A	566	LEU	2.4
1	B	576	GLU	2.4
1	B	945	LEU	2.3
1	A	942	ASP	2.3
1	C	546	LEU	2.3
1	A	577	ALA	2.3
1	B	658	PHE	2.3
1	B	571	ASP	2.3
1	C	917	ASP	2.3
1	C	850	VAL	2.3
1	C	566	LEU	2.3
1	A	660	GLY	2.3
1	C	743	ALA	2.2
1	C	445	LYS	2.2
1	A	661	ARG	2.2
1	B	479	VAL	2.2
1	B	561	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	887	GLU	2.2
1	C	640	ALA	2.2
1	B	585	SER	2.2
1	C	558	SER	2.2
1	C	677	ARG	2.2
1	C	555	VAL	2.2
1	B	786	THR	2.2
1	B	823	ARG	2.2
1	B	567	VAL	2.1
1	B	549	ALA	2.1
1	C	583	TYR	2.1
1	B	543	PRO	2.1
1	A	555	VAL	2.1
1	C	535	ALA	2.1
1	B	478	ARG	2.1
1	C	459	ARG	2.1
1	C	657	LEU	2.1
1	C	926	LEU	2.1
1	C	896	GLY	2.1
1	C	713	VAL	2.1
1	C	898	SER	2.1
1	C	937	SER	2.1
1	C	542	ARG	2.0
1	B	953	VAL	2.0
1	C	453	GLU	2.0
1	B	482	LEU	2.0
1	C	669	LEU	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( $\text{\AA}^2$ )	Q<0.9
3	AR6	C	1003	36/36	0.91	0.17	-0.25	23,40,50,51	0
3	AR6	A	1003	36/36	0.96	0.14	-0.38	24,34,41,44	0
3	AR6	B	1003	36/36	0.94	0.14	-0.58	26,38,47,52	0
2	IOD	A	1001	1/1	0.96	0.10	-1.97	78,78,78,78	0
2	IOD	C	1001	1/1	0.95	0.07	-3.49	98,98,98,98	0
2	IOD	B	1001	1/1	0.96	0.04	-4.19	75,75,75,75	0
2	IOD	C	1002	1/1	0.88	0.36	-	175,175,175,175	0
2	IOD	B	1002	1/1	0.96	0.09	-	93,93,93,93	0
2	IOD	A	1002	1/1	0.69	0.23	-	139,139,139,139	0

## 6.5 Other polymers

There are no such residues in this entry.