



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:18 am GMT

PDB ID : 1E90  
Title : STRUCTURE DETERMINANTS OF PHOSPHOINOSITIDE 3-KINASE INHIBITION BY WORTMANNIN, LY294002, QUERCETIN, MYRICETIN AND STAUROSPORINE  
Authors : Walker, E.H.; Pacold, M.E.; Perisic, O.; Stephens, L.; Hawkins, P.T.; Wymann, M.P.; Williams, R.L.  
Deposited on : 2000-10-03  
Resolution : 2.70 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

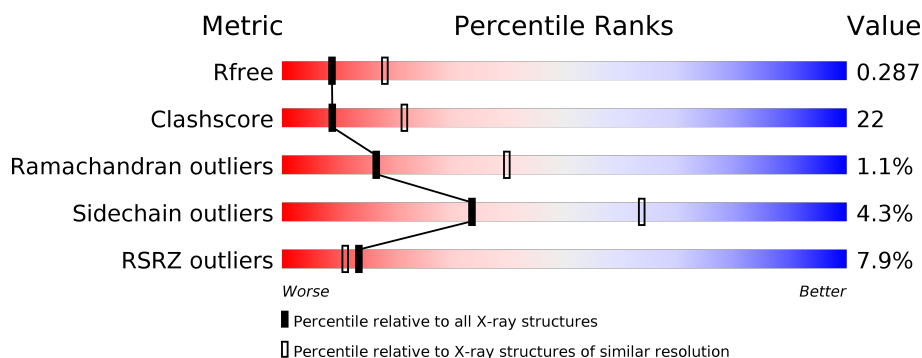
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	961	<div> <div>7%</div> <div>50%</div> <div>35%</div> <div>12%</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6862 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.

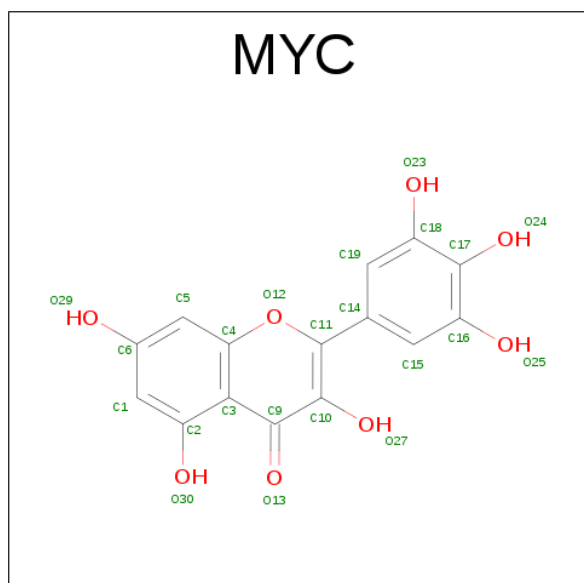
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	844	6839	4399	1160	1244	36	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	ALA	PRO	EXPRESSION TAG	UNP O02697
A	505	ALA	ARG	CONFLICT	UNP O02697

- Molecule 2 is 3,5,7-TRIHYDROXY-2-(3,4,5-TRIHYDROXYPHENYL)-4H-CHROMEN-4-ONE (three-letter code: MYC) (formula: C<sub>15</sub>H<sub>10</sub>O<sub>8</sub>).

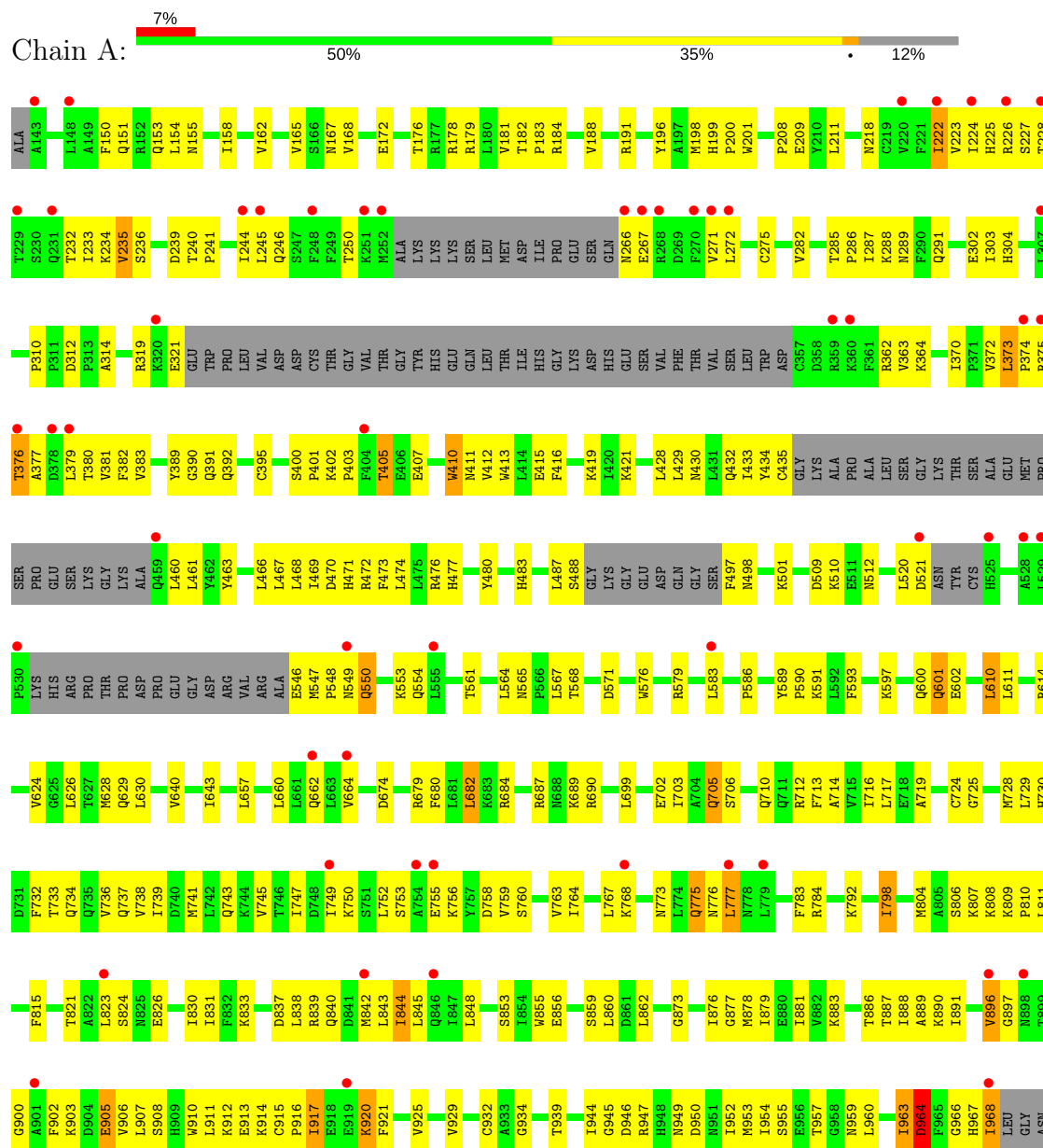


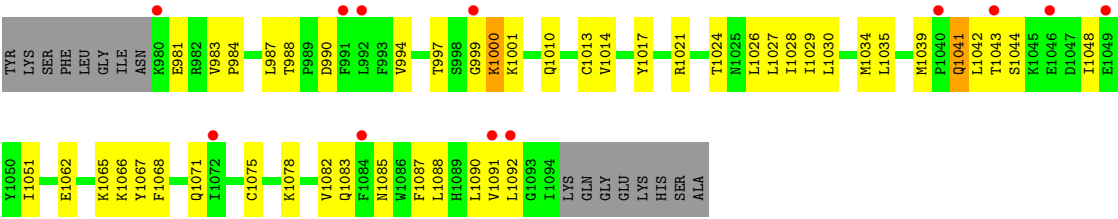
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	23	15	8	0	0

### 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 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: PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUBUNIT





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.68Å 67.73Å 106.99Å 90.00° 95.94° 90.00°	Depositor
Resolution (Å)	39.30 – 2.70 39.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.30-2.70) 99.1 (39.30-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.272 , 0.302 0.269 , 0.287	Depositor DCC
$R_{free}$ test set	1381 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.2	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 73.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYC

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	0.31	0/6981	0.53	0/9442

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

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	6839	0	6917	310	0
2	A	23	0	5	0	0
All	All	6862	0	6922	310	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 22.

All (310) 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:917:ILE:H	1:A:917:ILE:HD12	1.20	1.06
1:A:745:VAL:HG12	1:A:749:ILE:HD11	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:LYS:HD2	1:A:807:LYS:H	1.17	1.05
1:A:887:THR:HB	1:A:890:LYS:HG3	1.53	0.88
1:A:843:LEU:HD23	1:A:1034:MET:HG3	1.54	0.87
1:A:1035:LEU:HB3	1:A:1043:THR:HG21	1.56	0.85
1:A:241:PRO:HA	1:A:244:ILE:HD12	1.60	0.83
1:A:840:GLN:HE22	1:A:967:HIS:HA	1.43	0.83
1:A:807:LYS:HD2	1:A:807:LYS:N	1.94	0.81
1:A:917:ILE:HD13	1:A:920:LYS:HD2	1.62	0.81
1:A:1041:GLN:NE2	1:A:1041:GLN:H	1.78	0.80
1:A:611:LEU:O	1:A:614:ARG:HG3	1.82	0.80
1:A:561:THR:HG21	1:A:565:ASN:ND2	1.96	0.79
1:A:760:SER:O	1:A:763:VAL:HG12	1.81	0.79
1:A:549:ASN:OD1	1:A:553:LYS:HE3	1.83	0.79
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.48	0.77
1:A:497:PHE:HB3	1:A:1042:LEU:HB3	1.67	0.76
1:A:944:ILE:HG22	1:A:968:ILE:HD12	1.68	0.76
1:A:576:TRP:O	1:A:579:ARG:HG3	1.87	0.75
1:A:912:LYS:HG2	1:A:921:PHE:CE1	2.21	0.75
1:A:749:ILE:HD13	1:A:811:LEU:HD21	1.68	0.75
1:A:597:LYS:HD3	1:A:600:GLN:NE2	2.02	0.74
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.53	0.73
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.23	0.73
1:A:182:THR:HB	1:A:183:PRO:HD3	1.69	0.72
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.70	0.72
1:A:855:TRP:HB3	1:A:860:LEU:HB2	1.70	0.72
1:A:640:VAL:O	1:A:643:ILE:HG13	1.91	0.71
1:A:807:LYS:H	1:A:807:LYS:CD	1.99	0.70
1:A:747:ILE:HD11	1:A:876:ILE:HD13	1.73	0.70
1:A:921:PHE:O	1:A:925:VAL:HG23	1.91	0.70
1:A:184:ARG:O	1:A:188:VAL:HG23	1.94	0.68
1:A:777:LEU:O	1:A:777:LEU:HD23	1.94	0.68
1:A:739:ILE:O	1:A:743:GLN:HG2	1.93	0.67
1:A:222:ILE:HD13	1:A:222:ILE:H	1.59	0.67
1:A:629:GLN:HG2	1:A:1029:ILE:HD13	1.76	0.67
1:A:840:GLN:NE2	1:A:967:HIS:HA	2.09	0.67
1:A:917:ILE:HD13	1:A:920:LYS:CD	2.24	0.67
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.78	0.66
1:A:844:ILE:O	1:A:848:LEU:HD13	1.95	0.66
1:A:753:SER:HB3	1:A:809:LYS:NZ	2.11	0.66
1:A:914:LYS:C	1:A:916:PRO:HD3	2.15	0.66
1:A:887:THR:HB	1:A:890:LYS:CG	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:SER:O	1:A:912:LYS:HG3	1.95	0.66
1:A:244:ILE:HD11	1:A:287:ILE:CG2	2.26	0.65
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.96	0.65
1:A:550:GLN:O	1:A:550:GLN:NE2	2.24	0.65
1:A:1000:LYS:HE3	1:A:1000:LYS:HA	1.79	0.65
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.77	0.64
1:A:470:ASP:OD2	1:A:474:LEU:HB2	1.98	0.64
1:A:546:GLU:HG3	1:A:547:MET:N	2.12	0.64
1:A:917:ILE:H	1:A:917:ILE:CD1	1.98	0.64
1:A:402:LYS:HB3	1:A:403:PRO:HD2	1.79	0.64
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.80	0.64
1:A:501:LYS:NZ	1:A:501:LYS:HB3	2.13	0.64
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.12	0.63
1:A:747:ILE:HD11	1:A:876:ILE:CD1	2.28	0.63
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.81	0.63
1:A:597:LYS:HD3	1:A:600:GLN:HE22	1.64	0.62
1:A:917:ILE:N	1:A:917:ILE:HD12	2.04	0.62
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.30	0.62
1:A:487:LEU:HD23	1:A:488:SER:N	2.14	0.62
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.30	0.62
1:A:705:GLN:HE21	1:A:873:GLY:C	2.03	0.61
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.82	0.61
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.83	0.61
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.31	0.61
1:A:472:ARG:O	1:A:473:PHE:HB2	2.00	0.61
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.83	0.60
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.66	0.60
1:A:239:ASP:O	1:A:287:ILE:HG23	2.00	0.60
1:A:246:GLN:O	1:A:250:THR:HG23	2.02	0.60
1:A:275:CYS:HB3	1:A:823:LEU:HD13	1.83	0.60
1:A:564:LEU:HD21	1:A:1048:ILE:HG21	1.83	0.60
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.82	0.60
1:A:712:ARG:O	1:A:716:ILE:HD13	2.02	0.60
1:A:376:THR:HG23	1:A:376:THR:O	2.00	0.59
1:A:886:THR:HG22	1:A:887:THR:N	2.17	0.59
1:A:303:ILE:HD12	1:A:303:ILE:N	2.17	0.59
1:A:764:ILE:HG22	1:A:768:LYS:HE2	1.83	0.59
1:A:209:GLU:HB3	1:A:859:SER:HB3	1.85	0.59
1:A:165:VAL:O	1:A:165:VAL:HG12	2.03	0.59
1:A:947:ARG:NH1	1:A:964:ASP:O	2.27	0.59
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LEU:HD21	1:A:591:LYS:HD2	1.85	0.58
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.68	0.58
1:A:887:THR:HG22	1:A:889:ALA:H	1.68	0.58
1:A:200:PRO:HG3	1:A:282:VAL:HG23	1.84	0.58
1:A:939:THR:HG23	1:A:944:ILE:HG13	1.83	0.58
1:A:732:PHE:O	1:A:736:VAL:HG23	2.03	0.58
1:A:550:GLN:HE21	1:A:550:GLN:C	2.06	0.58
1:A:624:VAL:O	1:A:628:MET:HG2	2.03	0.58
1:A:946:ASP:O	1:A:947:ARG:HG2	2.04	0.57
1:A:810:PRO:HG3	1:A:833:LYS:HE3	1.85	0.57
1:A:831:ILE:HD11	1:A:881:ILE:HD11	1.86	0.57
1:A:235:VAL:HG12	1:A:239:ASP:OD2	2.03	0.57
1:A:843:LEU:CD2	1:A:1034:MET:HG3	2.29	0.57
1:A:981:GLU:OE1	1:A:1078:LYS:HE3	2.05	0.57
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.04	0.57
1:A:752:LEU:O	1:A:753:SER:HB3	2.05	0.57
1:A:233:ILE:N	1:A:233:ILE:HD12	2.20	0.57
1:A:477:HIS:O	1:A:480:TYR:HE1	1.88	0.56
1:A:725:GLY:O	1:A:729:LEU:HB2	2.05	0.56
1:A:755:GLU:HG2	1:A:755:GLU:O	2.05	0.56
1:A:753:SER:HB3	1:A:809:LYS:HZ2	1.70	0.56
1:A:469:ILE:N	1:A:469:ILE:HD12	2.19	0.56
1:A:568:THR:H	1:A:571:ASP:HB2	1.69	0.56
1:A:773:ASN:HA	1:A:776:ASN:ND2	2.21	0.56
1:A:703:ILE:HD11	1:A:714:ALA:N	2.21	0.56
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.88	0.56
1:A:839:ARG:HA	1:A:842:MET:HE2	1.89	0.55
1:A:910:TRP:O	1:A:914:LYS:HG2	2.06	0.55
1:A:498:ASN:ND2	1:A:1042:LEU:HD23	2.21	0.55
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.88	0.55
1:A:749:ILE:CD1	1:A:811:LEU:HD21	2.35	0.55
1:A:741:MET:O	1:A:745:VAL:HG23	2.06	0.55
1:A:745:VAL:O	1:A:749:ILE:HG13	2.06	0.55
1:A:963:ILE:O	1:A:964:ASP:C	2.44	0.55
1:A:903:LYS:HB3	1:A:905:GLU:OE1	2.06	0.55
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.36	0.55
1:A:244:ILE:HD11	1:A:287:ILE:HG21	1.88	0.54
1:A:915:CYS:HB3	1:A:920:LYS:HG2	1.88	0.54
1:A:939:THR:HG22	1:A:945:GLY:HA2	1.88	0.54
1:A:806:SER:HB3	1:A:810:PRO:HD3	1.90	0.54
1:A:364:LYS:HE2	1:A:411:ASN:OD1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:THR:HG23	1:A:1001:LYS:O	2.07	0.54
1:A:831:ILE:HB	1:A:879:ILE:HB	1.90	0.54
1:A:689:LYS:HG2	1:A:728:MET:CE	2.38	0.54
1:A:662:GLN:HE21	1:A:1030:LEU:HD22	1.74	0.53
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.91	0.53
1:A:509:ASP:OD2	1:A:512:ASN:HB2	2.08	0.53
1:A:826:GLU:HB3	1:A:883:LYS:HE2	1.90	0.53
1:A:225:HIS:CE1	1:A:823:LEU:HD21	2.43	0.53
1:A:837:ASP:OD1	1:A:839:ARG:HB2	2.09	0.53
1:A:840:GLN:O	1:A:844:ILE:HD13	2.09	0.53
1:A:657:LEU:HD11	1:A:690:ARG:HD3	1.91	0.52
1:A:743:GLN:O	1:A:747:ILE:HD13	2.08	0.52
1:A:381:VAL:HG12	1:A:435:CYS:HA	1.91	0.52
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.91	0.52
1:A:245:LEU:HD21	1:A:272:LEU:HG	1.90	0.52
1:A:240:THR:O	1:A:244:ILE:HG13	2.10	0.52
1:A:266:ASN:CG	1:A:267:GLU:H	2.12	0.52
1:A:705:GLN:NE2	1:A:873:GLY:O	2.43	0.52
1:A:749:ILE:HD13	1:A:767:LEU:HD23	1.91	0.52
1:A:887:THR:HG22	1:A:889:ALA:N	2.25	0.52
1:A:821:THR:HG22	1:A:821:THR:O	2.10	0.51
1:A:232:THR:C	1:A:233:ILE:HD12	2.31	0.51
1:A:1041:GLN:CD	1:A:1041:GLN:H	2.14	0.51
1:A:287:ILE:HD12	1:A:288:LYS:N	2.25	0.51
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.11	0.51
1:A:1088:LEU:HD23	1:A:1092:LEU:HD12	1.92	0.51
1:A:383:VAL:HG22	1:A:433:ILE:CD1	2.41	0.51
1:A:375:ARG:O	1:A:377:ALA:N	2.44	0.51
1:A:1062:GLU:O	1:A:1066:LYS:HD3	2.10	0.50
1:A:912:LYS:HE2	1:A:921:PHE:CZ	2.47	0.50
1:A:1024:THR:O	1:A:1028:ILE:HG12	2.11	0.50
1:A:228:THR:O	1:A:228:THR:HG22	2.10	0.50
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.27	0.50
1:A:932:CYS:HA	1:A:960:LEU:HD23	1.92	0.50
1:A:554:GLN:HA	1:A:554:GLN:NE2	2.26	0.50
1:A:1041:GLN:N	1:A:1041:GLN:NE2	2.54	0.50
1:A:602:GLU:H	1:A:602:GLU:CD	2.15	0.50
1:A:184:ARG:HH22	1:A:321:GLU:CD	2.15	0.50
1:A:784:ARG:HG2	1:A:784:ARG:HH11	1.77	0.49
1:A:660:LEU:O	1:A:664:VAL:HG23	2.11	0.49
1:A:162:VAL:HG12	1:A:714:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:VAL:HG12	1:A:897:GLY:N	2.27	0.49
1:A:497:PHE:HB3	1:A:1042:LEU:HD22	1.93	0.49
1:A:939:THR:HG21	1:A:945:GLY:HA2	1.94	0.49
1:A:372:VAL:HG12	1:A:373:LEU:N	2.28	0.49
1:A:379:LEU:HB3	1:A:435:CYS:SG	2.53	0.49
1:A:165:VAL:HG13	1:A:168:VAL:HG21	1.95	0.49
1:A:808:LYS:HD2	1:A:833:LYS:HE2	1.95	0.49
1:A:705:GLN:OE1	1:A:839:ARG:NE	2.46	0.48
1:A:303:ILE:HD12	1:A:303:ILE:H	1.77	0.48
1:A:806:SER:HB3	1:A:810:PRO:CD	2.43	0.48
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.12	0.48
1:A:165:VAL:HG13	1:A:168:VAL:CG2	2.43	0.48
1:A:223:VAL:HG12	1:A:225:HIS:CD2	2.48	0.48
1:A:747:ILE:HD12	1:A:747:ILE:N	2.29	0.48
1:A:853:SER:O	1:A:856:GLU:HB3	2.13	0.48
1:A:784:ARG:HG2	1:A:784:ARG:NH1	2.29	0.48
1:A:241:PRO:HA	1:A:244:ILE:CD1	2.40	0.48
1:A:200:PRO:HG3	1:A:282:VAL:CG2	2.44	0.48
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.14	0.48
1:A:589:TYR:HB2	1:A:590:PRO:HD3	1.95	0.48
1:A:167:ASN:O	1:A:168:VAL:HG13	2.14	0.47
1:A:370:ILE:O	1:A:370:ILE:HG23	2.14	0.47
1:A:188:VAL:O	1:A:191:ARG:HG2	2.15	0.47
1:A:419:LYS:HD3	1:A:421:LYS:HE2	1.95	0.47
1:A:886:THR:HG22	1:A:887:THR:H	1.79	0.47
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.79	0.47
1:A:428:LEU:HD23	1:A:467:LEU:HD23	1.95	0.47
1:A:549:ASN:O	1:A:553:LYS:HG3	2.15	0.47
1:A:756:LYS:HD3	1:A:756:LYS:HA	1.75	0.47
1:A:222:ILE:HD13	1:A:222:ILE:N	2.27	0.47
1:A:767:LEU:HD13	1:A:767:LEU:C	2.35	0.47
1:A:236:SER:HG	1:A:239:ASP:CG	2.18	0.47
1:A:501:LYS:HZ3	1:A:501:LYS:HB3	1.80	0.47
1:A:586:PRO:HA	1:A:589:TYR:CE1	2.50	0.47
1:A:702:GLU:O	1:A:706:SER:HB3	2.15	0.47
1:A:955:SER:C	1:A:957:THR:H	2.17	0.47
1:A:405:THR:HG23	1:A:407:GLU:O	2.15	0.47
1:A:1087:PHE:O	1:A:1091:VAL:HB	2.15	0.47
1:A:179:ARG:NH2	1:A:679:ARG:HH22	2.13	0.47
1:A:233:ILE:HG22	1:A:234:LYS:N	2.30	0.47
1:A:568:THR:N	1:A:571:ASP:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:GLN:HG3	1:A:1030:LEU:HD22	1.98	0.46
1:A:887:THR:HG21	1:A:950:ASP:OD1	2.16	0.46
1:A:750:LYS:HE3	1:A:808:LYS:HA	1.97	0.46
1:A:629:GLN:HG2	1:A:1029:ILE:CD1	2.45	0.46
1:A:876:ILE:HG22	1:A:877:GLY:N	2.30	0.46
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.50	0.46
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.31	0.46
1:A:783:PHE:N	1:A:792:LYS:HE2	2.30	0.46
1:A:687:ARG:HG2	1:A:687:ARG:O	2.16	0.45
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.52	0.45
1:A:151:GLN:HG3	1:A:155:ASN:HD21	1.80	0.45
1:A:362:ARG:HB3	1:A:415:GLU:HG3	1.99	0.45
1:A:643:ILE:C	1:A:643:ILE:HD12	2.36	0.45
1:A:389:TYR:O	1:A:392:GLN:HG2	2.17	0.45
1:A:196:TYR:OH	1:A:728:MET:HE2	2.16	0.45
1:A:954:ILE:HD12	1:A:959:ASN:C	2.37	0.45
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.52	0.45
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.52	0.45
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.45	0.45
1:A:946:ASP:C	1:A:947:ARG:HG2	2.37	0.45
1:A:734:GLN:O	1:A:738:VAL:HG23	2.16	0.45
1:A:939:THR:HG22	1:A:945:GLY:CA	2.47	0.45
1:A:844:ILE:CD1	1:A:844:ILE:N	2.79	0.45
1:A:271:VAL:HG22	1:A:272:LEU:N	2.32	0.44
1:A:763:VAL:HG13	1:A:764:ILE:N	2.32	0.44
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.47	0.44
1:A:286:PRO:HD2	1:A:289:ASN:HD22	1.80	0.44
1:A:1000:LYS:HE3	1:A:1000:LYS:CA	2.48	0.44
1:A:703:ILE:HD11	1:A:713:PHE:CB	2.46	0.44
1:A:730:HIS:O	1:A:734:GLN:HG2	2.17	0.44
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.99	0.44
1:A:181:VAL:HG13	1:A:184:ARG:NH2	2.33	0.44
1:A:150:PHE:CE1	1:A:319:ARG:HD3	2.52	0.44
1:A:380:THR:O	1:A:435:CYS:HA	2.18	0.44
1:A:287:ILE:C	1:A:287:ILE:HD12	2.38	0.44
1:A:699:LEU:O	1:A:703:ILE:HG12	2.18	0.44
1:A:815:PHE:CE1	1:A:830:ILE:HD12	2.52	0.44
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.53	0.43
1:A:498:ASN:C	1:A:498:ASN:OD1	2.57	0.43
1:A:824:SER:OG	1:A:826:GLU:HG3	2.17	0.43
1:A:804:MET:HE2	1:A:831:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:HD22	1:A:610:LEU:HD21	2.00	0.43
1:A:804:MET:C	1:A:806:SER:H	2.22	0.43
1:A:410:TRP:HB3	1:A:412:VAL:HG23	1.99	0.43
1:A:888:ILE:HA	1:A:891:ILE:HD12	2.00	0.43
1:A:862:LEU:HD12	1:A:934:GLY:HA2	2.00	0.43
1:A:1044:SER:O	1:A:1048:ILE:HG12	2.19	0.43
1:A:382:PHE:CE1	1:A:434:TYR:HB2	2.54	0.43
1:A:364:LYS:HD2	1:A:413:TRP:CE2	2.54	0.43
1:A:225:HIS:HE1	1:A:823:LEU:HD21	1.82	0.43
1:A:886:THR:CG2	1:A:887:THR:N	2.82	0.43
1:A:419:LYS:CD	1:A:421:LYS:HE2	2.49	0.42
1:A:953:MET:HG3	1:A:963:ILE:HD13	2.01	0.42
1:A:990:ASP:O	1:A:994:VAL:HG23	2.19	0.42
1:A:967:HIS:O	1:A:968:ILE:O	2.38	0.42
1:A:150:PHE:O	1:A:153:GLN:HG2	2.20	0.42
1:A:497:PHE:CB	1:A:1042:LEU:HD22	2.49	0.42
1:A:905:GLU:N	1:A:905:GLU:OE1	2.37	0.42
1:A:1083:GLN:HA	1:A:1083:GLN:NE2	2.34	0.42
1:A:285:THR:HG22	1:A:289:ASN:HB2	2.02	0.42
1:A:223:VAL:HG12	1:A:225:HIS:NE2	2.34	0.42
1:A:400:SER:HA	1:A:401:PRO:HD3	1.94	0.42
1:A:745:VAL:HG12	1:A:749:ILE:CD1	2.24	0.42
1:A:225:HIS:N	1:A:225:HIS:CD2	2.88	0.42
1:A:178:ARG:O	1:A:181:VAL:HG23	2.19	0.42
1:A:568:THR:H	1:A:571:ASP:CB	2.31	0.42
1:A:753:SER:HB3	1:A:809:LYS:HZ1	1.81	0.42
1:A:154:LEU:O	1:A:158:ILE:HG13	2.20	0.42
1:A:435:CYS:HB2	1:A:461:LEU:HD12	2.02	0.42
1:A:798:ILE:HG13	1:A:798:ILE:H	1.69	0.41
1:A:967:HIS:O	1:A:968:ILE:C	2.58	0.41
1:A:497:PHE:CB	1:A:1042:LEU:HB3	2.45	0.41
1:A:952:ILE:CG2	1:A:960:LEU:HD11	2.50	0.41
1:A:266:ASN:CG	1:A:267:GLU:N	2.72	0.41
1:A:162:VAL:CG1	1:A:714:ALA:HB1	2.50	0.41
1:A:896:VAL:HG12	1:A:897:GLY:H	1.85	0.41
1:A:999:GLY:C	1:A:1001:LYS:H	2.23	0.41
1:A:831:ILE:O	1:A:878:MET:HA	2.21	0.41
1:A:601:GLN:HG3	1:A:602:GLU:N	2.35	0.41
1:A:165:VAL:O	1:A:165:VAL:CG1	2.69	0.41
1:A:373:LEU:HB2	1:A:374:PRO:CD	2.50	0.41
1:A:430:ASN:OD1	1:A:432:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:HB	1:A:310:PRO:HG3	2.03	0.41
1:A:682:LEU:HD11	1:A:719:ALA:HB1	2.03	0.41
1:A:1088:LEU:O	1:A:1092:LEU:HB2	2.21	0.41
1:A:390:GLY:O	1:A:391:GLN:HB3	2.21	0.41
1:A:630:LEU:CD1	1:A:643:ILE:HD11	2.51	0.41
1:A:900:GLY:O	1:A:902:PHE:N	2.47	0.41
1:A:224:ILE:HD12	1:A:272:LEU:CD2	2.51	0.41
1:A:987:LEU:HB3	1:A:1075:CYS:HB3	2.03	0.40
1:A:373:LEU:HB2	1:A:374:PRO:HD2	2.02	0.40
1:A:775:GLN:O	1:A:776:ASN:C	2.57	0.40
1:A:198:MET:O	1:A:199:HIS:C	2.60	0.40
1:A:520:LEU:O	1:A:521:ASP:C	2.59	0.40
1:A:703:ILE:HD13	1:A:710:GLN:HA	2.02	0.40
1:A:831:ILE:CD1	1:A:881:ILE:HD11	2.50	0.40
1:A:988:THR:HG21	1:A:1083:GLN:HG3	2.03	0.40
1:A:1082:VAL:O	1:A:1085:ASN:HB2	2.21	0.40
1:A:467:LEU:O	1:A:476:ARG:HD2	2.21	0.40
1:A:680:PHE:O	1:A:684:ARG:HG2	2.22	0.40
1:A:483:HIS:CD2	1:A:510:LYS:HG2	2.57	0.40
1:A:925:VAL:O	1:A:929:VAL:HG23	2.21	0.40
1:A:983:VAL:HG22	1:A:984:PRO:CD	2.50	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	828/961 (86%)	752 (91%)	67 (8%)	9 (1%)	17	40

All (9) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	896	VAL
1	A	966	GLY
1	A	758	ASP
1	A	777	LEU
1	A	964	ASP
1	A	963	ILE
1	A	376	THR
1	A	798	ILE
1	A	759	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	761/857 (89%)	728 (96%)	33 (4%)	33 64

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	222	ILE
1	A	226	ARG
1	A	227	SER
1	A	235	VAL
1	A	373	LEU
1	A	395	CYS
1	A	405	THR
1	A	410	TRP
1	A	548	PRO
1	A	550	GLN
1	A	601	GLN
1	A	610	LEU
1	A	626	LEU
1	A	682	LEU
1	A	705	GLN
1	A	717	LEU
1	A	775	GLN

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Mol	Chain	Res	Type
1	A	844	ILE
1	A	845	LEU
1	A	905	GLU
1	A	907	LEU
1	A	911	LEU
1	A	913	GLU
1	A	917	ILE
1	A	920	LYS
1	A	964	ASP
1	A	968	ILE
1	A	1000	LYS
1	A	1026	LEU
1	A	1027	LEU
1	A	1041	GLN
1	A	1090	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	304	HIS
1	A	396	GLN
1	A	459	GLN
1	A	550	GLN
1	A	554	GLN
1	A	565	ASN
1	A	600	GLN
1	A	601	GLN
1	A	639	ASN
1	A	708	HIS
1	A	710	GLN
1	A	737	GLN
1	A	776	ASN
1	A	778	ASN
1	A	840	GLN
1	A	922	GLN
1	A	951	ASN
1	A	1007	GLN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN
1	A	1089	HIS

### 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 ⓘ

1 ligand is 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	MYC	A	2095	-	23,25,25	1.86	4 (17%)	29,38,38	1.49	4 (13%)

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	MYC	A	2095	-	-	0/4/4/4	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	MYC	C14-C11	3.01	1.51	1.46
2	A	2095	MYC	C15-C16	3.06	1.43	1.38
2	A	2095	MYC	C1-C6	3.84	1.45	1.39
2	A	2095	MYC	C9-C3	4.26	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2095	MYC	C10-C9-C3	-3.19	116.86	121.28
2	A	2095	MYC	C18-C17-C16	-2.02	118.21	119.50
2	A	2095	MYC	C19-C18-C17	2.45	122.13	120.45
2	A	2095	MYC	C14-C11-C10	4.50	128.35	120.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	844/961 (87%)	0.52	67 (7%) 13 11	27, 72, 128, 184	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	529	LEU	6.6
1	A	248	PHE	5.8
1	A	375	ARG	5.3
1	A	245	LEU	5.3
1	A	898	ASN	4.9
1	A	252	MET	4.6
1	A	777	LEU	4.1
1	A	148	LEU	4.1
1	A	919	GLU	4.1
1	A	530	PRO	4.1
1	A	307	LEU	3.9
1	A	226	ARG	3.9
1	A	272	LEU	3.8
1	A	754	ALA	3.8
1	A	549	ASN	3.7
1	A	224	ILE	3.7
1	A	404	PHE	3.5
1	A	374	PRO	3.5
1	A	896	VAL	3.4
1	A	270	PHE	3.4
1	A	749	ILE	3.3
1	A	266	ASN	3.3
1	A	228	THR	3.2
1	A	231	GLN	3.0
1	A	251	LYS	3.0
1	A	525	HIS	3.0
1	A	379	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	229	THR	2.9
1	A	222	ILE	2.9
1	A	268	ARG	2.8
1	A	664	VAL	2.7
1	A	528	ALA	2.7
1	A	1092	LEU	2.7
1	A	271	VAL	2.7
1	A	1043	THR	2.7
1	A	901	ALA	2.7
1	A	823	LEU	2.7
1	A	244	ILE	2.6
1	A	999	GLY	2.5
1	A	521	ASP	2.5
1	A	662	GLN	2.4
1	A	267	GLU	2.4
1	A	1046	GLU	2.4
1	A	846	GLN	2.4
1	A	768	LYS	2.4
1	A	220	VAL	2.3
1	A	755	GLU	2.3
1	A	1084	PHE	2.3
1	A	378	ASP	2.3
1	A	1091	VAL	2.3
1	A	555	LEU	2.3
1	A	992	LEU	2.3
1	A	320	LYS	2.3
1	A	842	MET	2.2
1	A	968	ILE	2.2
1	A	143	ALA	2.2
1	A	991	PHE	2.2
1	A	376	THR	2.2
1	A	1040	PRO	2.2
1	A	980	LYS	2.1
1	A	360	LYS	2.1
1	A	1072	ILE	2.1
1	A	1049	GLU	2.1
1	A	779	LEU	2.1
1	A	583	LEU	2.0
1	A	359	ARG	2.0
1	A	459	GLN	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
2	MYC	A	2095	23/23	0.84	0.28	1.39	93,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.