



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:45 PM UTC

PDB ID : 1E90 / pdb_00001e90
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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

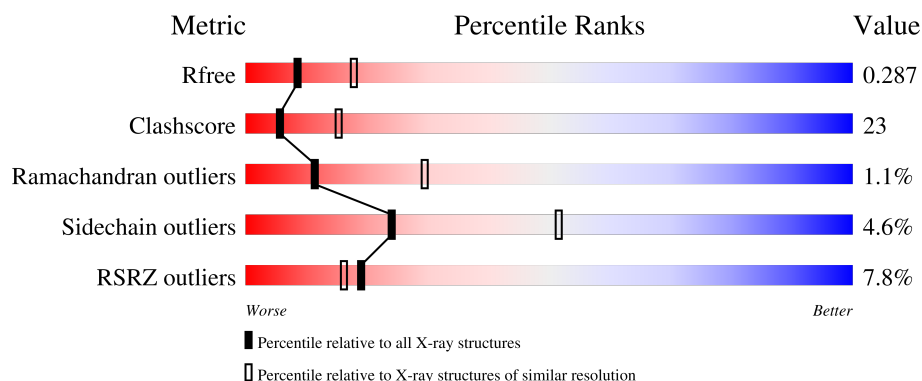
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	961	7% 49% 36% • 12%

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.

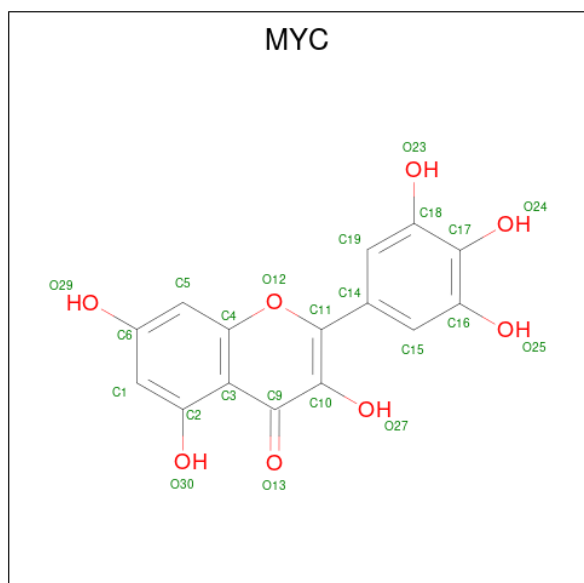
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

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 (CCD ID: MYC) (formula: C₁₅H₁₀O₈).

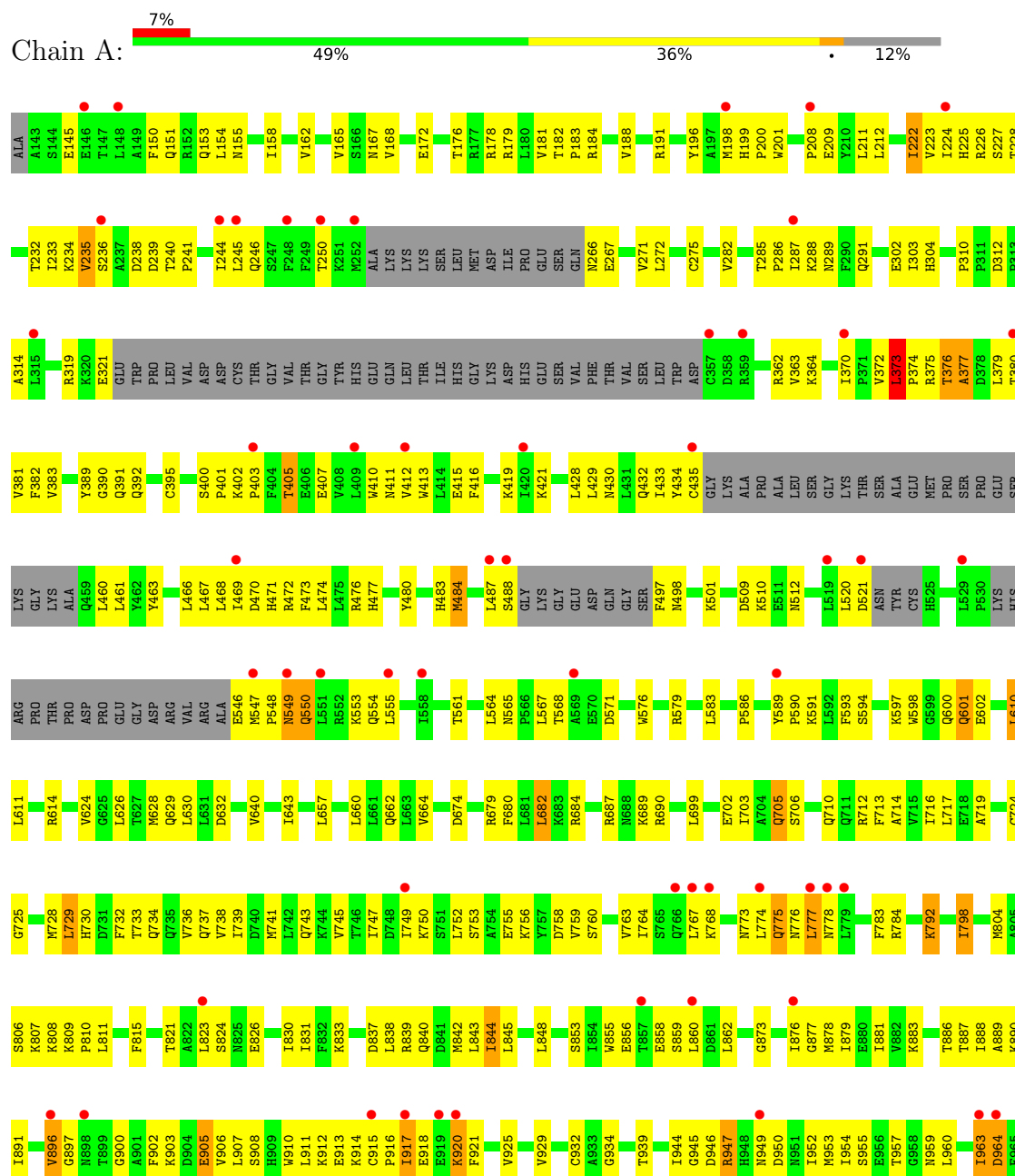


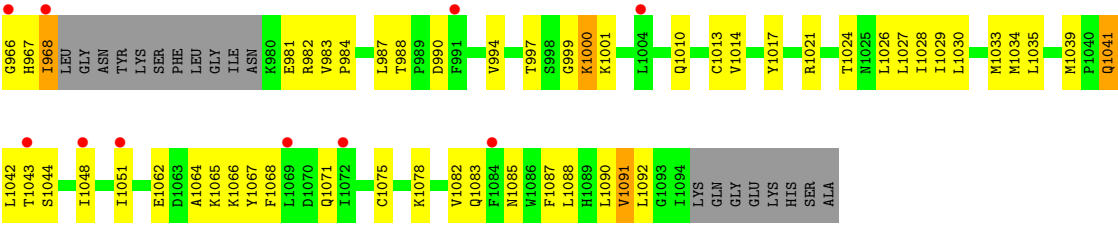
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	23	15	8	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 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, α , β , γ	143.68Å 67.73Å 106.99Å 90.00° 95.94° 90.00°	Depositor
Resolution (Å)	39.30 – 2.70 39.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.30-2.70) 99.0 (39.30-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	1541 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6862	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.36	0/6981	0.84	8/9442 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ALA	N-CA-C	8.24	122.11	112.72
1	A	373	LEU	CA-C-N	7.52	127.53	119.78
1	A	373	LEU	C-N-CA	7.52	127.53	119.78
1	A	484	MET	N-CA-C	6.14	117.97	110.41
1	A	947	ARG	N-CA-C	5.95	118.46	109.23
1	A	594	SER	N-CA-C	-5.86	106.18	113.38
1	A	1091	VAL	N-CA-C	5.66	116.44	110.72
1	A	549	ASN	N-CA-C	5.03	116.77	111.28

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	6839	0	6917	323	0
2	A	23	0	5	0	0
All	All	6862	0	6922	323	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 23.

All (323) 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:HD12	1:A:917:ILE:H	1.20	1.06
1:A:745:VAL:HG12	1:A:749:ILE:HD11	1.33	1.05
1:A:807:LYS:H	1:A:807:LYS:HD2	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:H	1:A:1041:GLN:NE2	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:433:ILE:HG12	1:A:484:MET:HE1	1.70	0.74
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:914:LYS:C	1:A:916:PRO:HD3	2.15	0.71
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:HD23	1:A:777:LEU:O	1.94	0.68
1:A:739:ILE:O	1:A:743:GLN:HG2	1.93	0.67
1:A:222:ILE:H	1:A:222:ILE:HD13	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:705:GLN:HE21	1:A:873:GLY:C	2.03	0.66
1:A:887:THR:HB	1:A:890:LYS:CG	2.25	0.66
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:753:SER:HB3	1:A:809:LYS:HZ2	1.63	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:550:GLN:HE21	1:A:550:GLN:C	2.06	0.63
1:A:597:LYS:HD3	1:A:600:GLN:HE22	1.64	0.62
1:A:917:ILE:HD12	1:A:917:ILE:N	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: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:501:LYS:HB3	1:A:501:LYS:HZ2	1.66	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:804:MET:HE3	1:A:810:PRO:HB2	1.82	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD21	1:A:1048:ILE:HG21	1.83	0.60
1:A:963:ILE:O	1:A:964:ASP:C	2.44	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:HG12	1:A:165:VAL:O	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
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:724:CYS:HB2	1:A:728:MET:HE3	1.85	0.58
1:A:732:PHE:O	1:A:736:VAL:HG23	2.03	0.58
1:A:839:ARG:HA	1:A:842:MET:HE2	1.84	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:752:LEU:O	1:A:753:SER:HB3	2.05	0.57
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.04	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:266:ASN:CG	1:A:267:GLU:H	2.12	0.56
1:A:755:GLU:HG2	1:A:755:GLU:O	2.05	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:232:THR:C	1:A:233:ILE:HD12	2.31	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:1041:GLN:H	1:A:1041:GLN:CD	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:602:GLU:CD	1:A:602:GLU:H	2.15	0.55
1:A:184:ARG:HH22	1:A:321:GLU:CD	2.15	0.54
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:804:MET:HE1	1:A:831:ILE:HD13	1.89	0.54
1:A:364:LYS:HE2	1:A:411:ASN:OD1	2.06	0.54
1:A:831:ILE:HB	1:A:879:ILE:HB	1.90	0.54
1:A:997:THR:HG23	1:A:1001:LYS:O	2.07	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:236:SER:HG	1:A:239:ASP:CG	2.16	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:1035:LEU:HD12	1:A:1048:ILE:HD13	1.91	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:245:LEU:HD21	1:A:272:LEU:HG	1.90	0.52
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.91	0.52
1:A:240:THR:O	1:A:244:ILE:HG13	2.10	0.52
1:A:767:LEU:HD13	1:A:767:LEU:C	2.35	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:955:SER:C	1:A:957:THR:H	2.17	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:383:VAL:HG22	1:A:433:ILE:CD1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:LEU:HD23	1:A:1092:LEU:HD12	1.92	0.51
1:A:375:ARG:O	1:A:377:ALA:N	2.44	0.51
1:A:547:MET:HE1	1:A:555:LEU:HD22	1.93	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:954:ILE:HD12	1:A:959:ASN:C	2.37	0.50
1:A:228:THR:O	1:A:228:THR:HG22	2.10	0.50
1:A:1024:THR:O	1:A:1028:ILE:HG12	2.11	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:643:ILE:C	1:A:643:ILE:HD12	2.36	0.50
1:A:741:MET:HE2	1:A:774:LEU:HD22	1.93	0.50
1:A:1041:GLN:NE2	1:A:1041:GLN:N	2.54	0.50
1:A:946:ASP:C	1:A:947:ARG:HG2	2.37	0.50
1:A:784:ARG:HH11	1:A:784:ARG:HG2	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
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:632:ASP:HB3	1:A:1033:MET:HE3	1.95	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:287:ILE:HD12	1:A:287:ILE:C	2.38	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: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:1067:TYR:O	1:A:1071:GLN:HG2	2.12	0.48
1:A:498:ASN:OD1	1:A:498:ASN:C	2.57	0.48
1:A:784:ARG:HG2	1:A:784:ARG:NH1	2.29	0.48
1:A:804:MET:C	1:A:806:SER:H	2.22	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:589:TYR:HB2	1:A:590:PRO:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.14	0.48
1:A:167:ASN:O	1:A:168:VAL:HG13	2.14	0.47
1:A:370:ILE:HG23	1:A:370:ILE:O	2.14	0.47
1:A:188:VAL:O	1:A:191:ARG:HG2	2.15	0.47
1:A:266:ASN:CG	1:A:267:GLU:N	2.72	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:HA	1:A:756:LYS:HD3	1.75	0.47
1:A:222:ILE:HD13	1:A:222:ILE:N	2.27	0.47
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.97	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:405:THR:HG23	1:A:407:GLU:O	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
1:A:1087:PHE:O	1:A:1091:VAL:HB	2.15	0.47
1:A:662:GLN:HG3	1:A:1030:LEU:HD22	1.98	0.46
1:A:967:HIS:O	1:A:968:ILE:C	2.58	0.46
1:A:887:THR:HG21	1:A:950:ASP:OD1	2.16	0.46
1:A:999:GLY:C	1:A:1001:LYS:H	2.23	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:O	1:A:687:ARG:HG2	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:196:TYR:OH	1:A:728:MET:HE2	2.17	0.45
1:A:362:ARG:HB3	1:A:415:GLU:HG3	1.99	0.45
1:A:520:LEU:O	1:A:521:ASP:C	2.59	0.45
1:A:775:GLN:O	1:A:776:ASN:C	2.57	0.45
1:A:198:MET:O	1:A:199:HIS:C	2.60	0.45
1:A:389:TYR:O	1:A:392:GLN:HG2	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.45	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:286:PRO:HD2	1:A:289:ASN:HD22	1.80	0.44
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.47	0.44
1:A:703:ILE:HD11	1:A:713:PHE:CB	2.46	0.44
1:A:1000:LYS:HE3	1:A:1000:LYS:CA	2.48	0.44
1:A:598:TRP:C	1:A:600:GLN:H	2.26	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:150:PHE:CE1	1:A:319:ARG:HD3	2.52	0.44
1:A:181:VAL:HG13	1:A:184:ARG:NH2	2.33	0.44
1:A:380:THR:O	1:A:435:CYS:HA	2.18	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:824:SER:OG	1:A:826:GLU:HG3	2.17	0.43
1:A:236:SER:C	1:A:238:ASP:H	2.25	0.43
1:A:583:LEU:HD22	1:A:610:LEU:HD21	2.00	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:382:PHE:CE1	1:A:434:TYR:HB2	2.54	0.43
1:A:1044:SER:O	1:A:1048:ILE:HG12	2.19	0.43
1:A:225:HIS:HE1	1:A:823:LEU:HD21	1.82	0.43
1:A:364:LYS:HD2	1:A:413:TRP:CE2	2.54	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:OE1	1:A:905:GLU:N	2.37	0.42
1:A:285:THR:HG22	1:A:289:ASN:HB2	2.02	0.42
1:A:705:GLN:NE2	1:A:873:GLY:C	2.74	0.42
1:A:1083:GLN:NE2	1:A:1083:GLN:HA	2.34	0.42
1:A:223:VAL:HG12	1:A:225:HIS:NE2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD2	1:A:225:HIS:N	2.88	0.42
1:A:1064:ALA:O	1:A:1065:LYS:C	2.62	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: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:981:GLU:C	1:A:982:ARG:HG3	2.44	0.42
1:A:798:ILE:H	1:A:798:ILE:HG13	1.69	0.41
1:A:497:PHE:CB	1:A:1042:LEU:HB3	2.45	0.41
1:A:741:MET:HE3	1:A:778:ASN:ND2	2.35	0.41
1:A:952:ILE:CG2	1:A:960:LEU:HD11	2.50	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: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
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:918:GLU:C	1:A:920:LYS:N	2.78	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:1088:LEU:O	1:A:1092:LEU:HB2	2.21	0.41
1:A:224:ILE:HD12	1:A:272:LEU:CD2	2.51	0.41
1:A:373:LEU:HB2	1:A:374:PRO:HD2	2.02	0.40
1:A:987:LEU:HB3	1:A:1075:CYS:HB3	2.03	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: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:1082:VAL:O	1:A:1085:ASN:HB2	2.21	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
1:A:1087:PHE:CD1	1:A:1087:PHE:C	3.00	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%)	11	29

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 [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	761/857 (89%)	726 (95%)	35 (5%)	24	51

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	212	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	729	LEU
1	A	775	GLN
1	A	792	LYS
1	A	844	ILE
1	A	845	LEU
1	A	858	GLU
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	968	ILE
1	A	1000	LYS
1	A	1026	LEU
1	A	1027	LEU
1	A	1041	GLN
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	A	299	ASN
1	A	304	HIS
1	A	391	GLN
1	A	396	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	459	GLN
1	A	550	GLN
1	A	554	GLN
1	A	565	ASN
1	A	600	GLN
1	A	629	GLN
1	A	639	ASN
1	A	662	GLN
1	A	708	HIS
1	A	710	GLN
1	A	730	HIS
1	A	737	GLN
1	A	776	ASN
1	A	778	ASN
1	A	840	GLN
1	A	922	GLN
1	A	1007	GLN
1	A	1023	HIS
1	A	1025	ASN
1	A	1041	GLN
1	A	1083	GLN
1	A	1085	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](#)

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	-	25,25,25	1.81	6 (24%)	38,38,38	1.14	4 (10%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	MYC	C10-C11	4.33	1.40	1.36
2	A	2095	MYC	C1-C6	3.96	1.45	1.39
2	A	2095	MYC	C15-C16	2.95	1.43	1.38
2	A	2095	MYC	C14-C11	2.79	1.51	1.47
2	A	2095	MYC	C3-C2	2.61	1.45	1.41
2	A	2095	MYC	C19-C14	2.14	1.42	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2095	MYC	O27-C10-C11	2.46	123.29	120.74
2	A	2095	MYC	C19-C18-C17	2.42	122.13	120.45
2	A	2095	MYC	C2-C3-C9	2.15	124.63	121.45
2	A	2095	MYC	C18-C17-C16	-2.14	118.21	119.53

There are no chirality outliers.

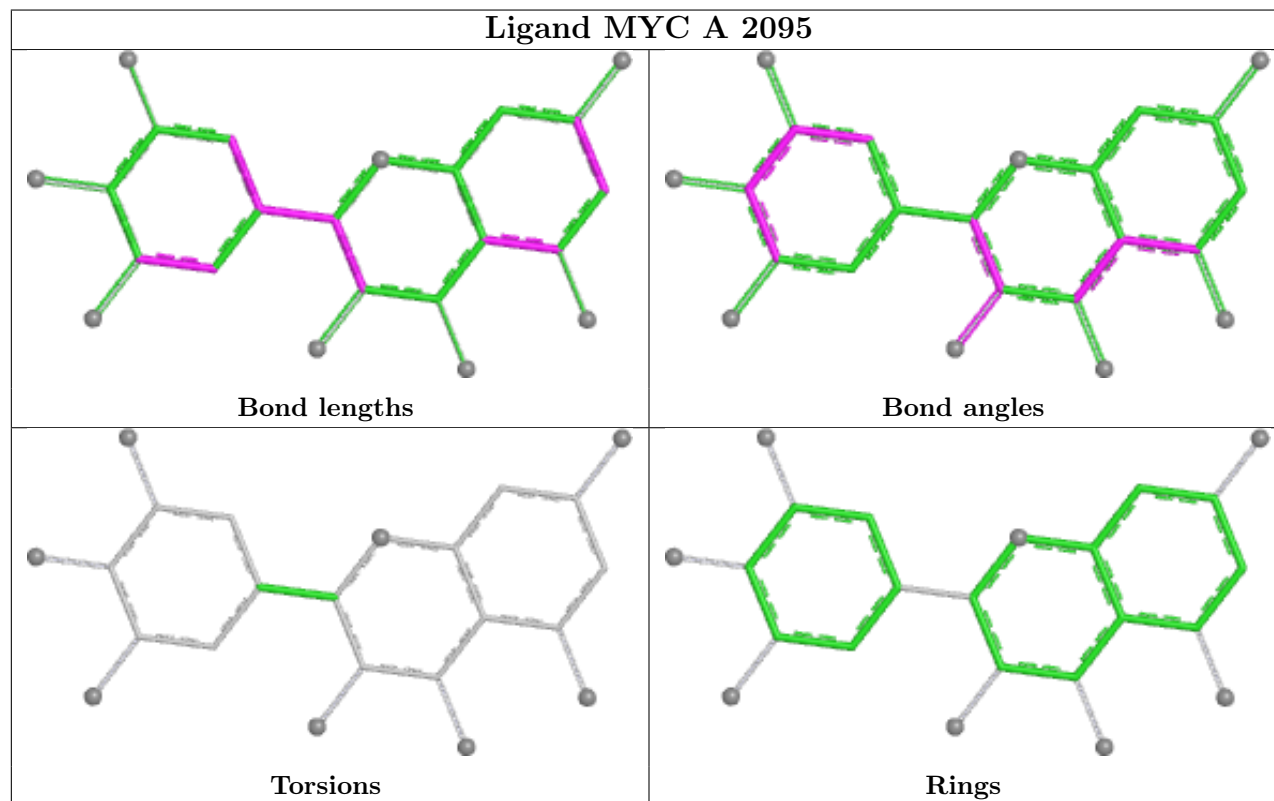
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	844/961 (87%)	0.72	66 (7%) 19 16	27, 72, 128, 184	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	966	GLY	4.8
1	A	917	ILE	4.2
1	A	521	ASP	4.0
1	A	968	ILE	4.0
1	A	403	PRO	4.0
1	A	749	ILE	3.7
1	A	1004	LEU	3.2
1	A	555	LEU	3.2
1	A	519	LEU	3.2
1	A	777	LEU	3.2
1	A	357	CYS	3.2
1	A	529	LEU	3.1
1	A	244	ILE	3.1
1	A	915	CYS	3.0
1	A	991	PHE	2.9
1	A	768	LYS	2.9
1	A	919	GLU	2.9
1	A	964	ASP	2.9
1	A	896	VAL	2.8
1	A	208	PRO	2.7
1	A	779	LEU	2.7
1	A	248	PHE	2.7
1	A	420	ILE	2.7
1	A	963	ILE	2.7
1	A	547	MET	2.6
1	A	549	ASN	2.6
1	A	949	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	766	GLN	2.6
1	A	1072	ILE	2.6
1	A	287	ILE	2.5
1	A	1048	ILE	2.5
1	A	767	LEU	2.5
1	A	774	LEU	2.5
1	A	245	LEU	2.5
1	A	409	LEU	2.5
1	A	148	LEU	2.5
1	A	876	ILE	2.5
1	A	778	ASN	2.4
1	A	146	GLU	2.4
1	A	488	SER	2.4
1	A	224	ILE	2.3
1	A	1043	THR	2.3
1	A	1051	ILE	2.3
1	A	359	ARG	2.3
1	A	920	LYS	2.2
1	A	380	THR	2.2
1	A	558	ILE	2.2
1	A	1084	PHE	2.2
1	A	435	CYS	2.2
1	A	250	THR	2.2
1	A	857	THR	2.2
1	A	569	ALA	2.2
1	A	898	ASN	2.2
1	A	823	LEU	2.2
1	A	252	MET	2.2
1	A	412	VAL	2.2
1	A	1069	LEU	2.1
1	A	370	ILE	2.1
1	A	236	SER	2.1
1	A	198	MET	2.0
1	A	315	LEU	2.0
1	A	487	LEU	2.0
1	A	551	LEU	2.0
1	A	860	LEU	2.0
1	A	589	TYR	2.0
1	A	469	ILE	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](#)

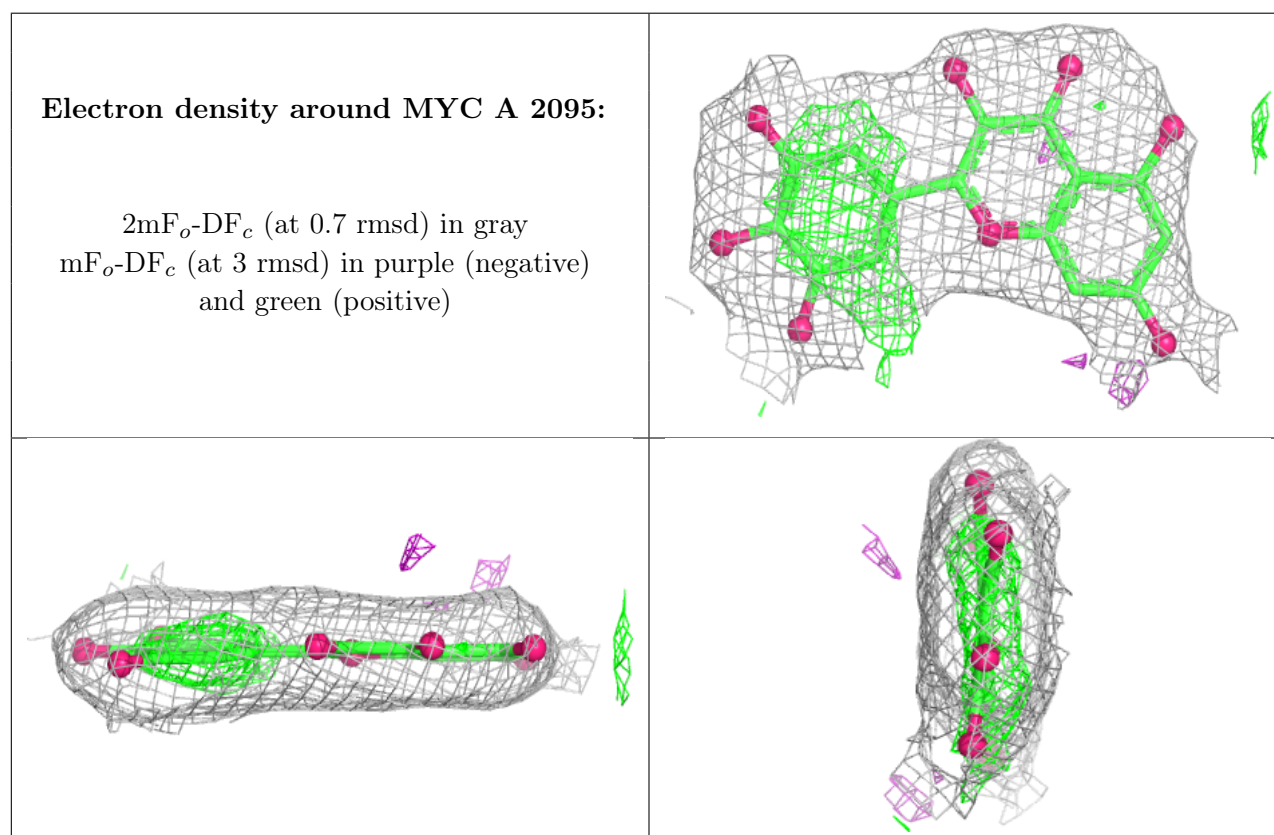
There are no oligosaccharides in this entry.

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	MYC	A	2095	23/23	0.87	0.18	93,93,93,93	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.