



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:16 pm BST

PDB ID : 1E7V  
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 : 2000-09-08  
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

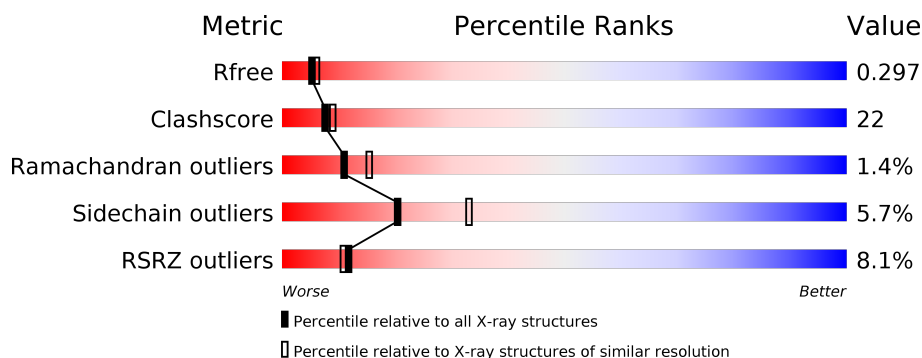
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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	<div> <div>7%</div> <div> <div></div> <div>48%</div> <div>37%</div> <div>•</div> <div>12%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7047 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.

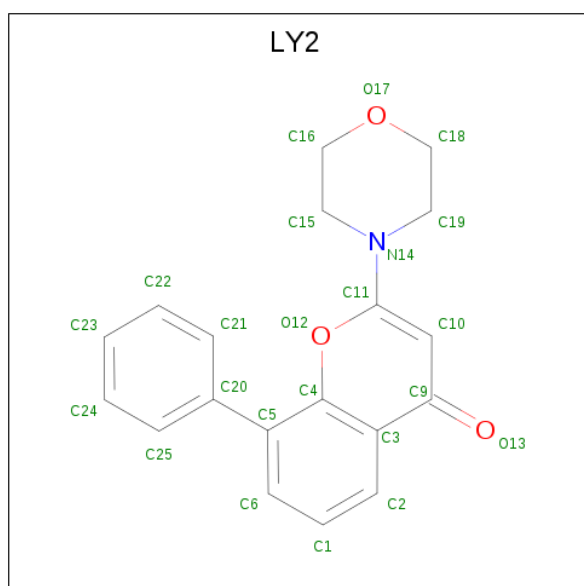
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	0	0
			6889	4434	1166	1252	37			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ALA	-	expression tag	UNP O02697
A	143	ALA	-	expression tag	UNP O02697
A	505	ALA	ARG	conflict	UNP O02697

- Molecule 2 is 2-MORPHOLIN-4-YL-7-PHENYL-4H-CHROMEN-4-ONE (three-letter code: LY2) (formula: C<sub>19</sub>H<sub>17</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	19	1	3		

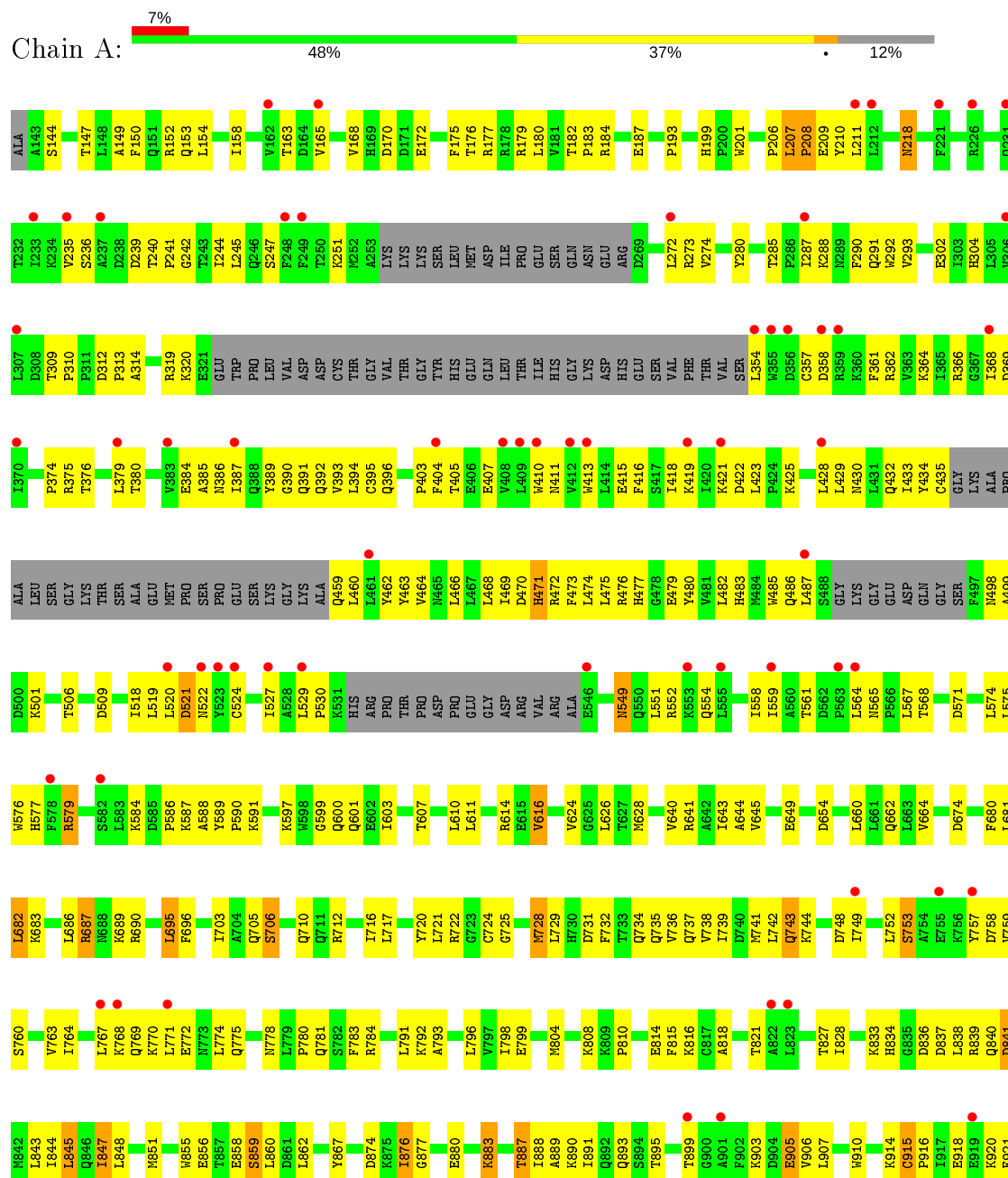
- Molecule 3 is water.

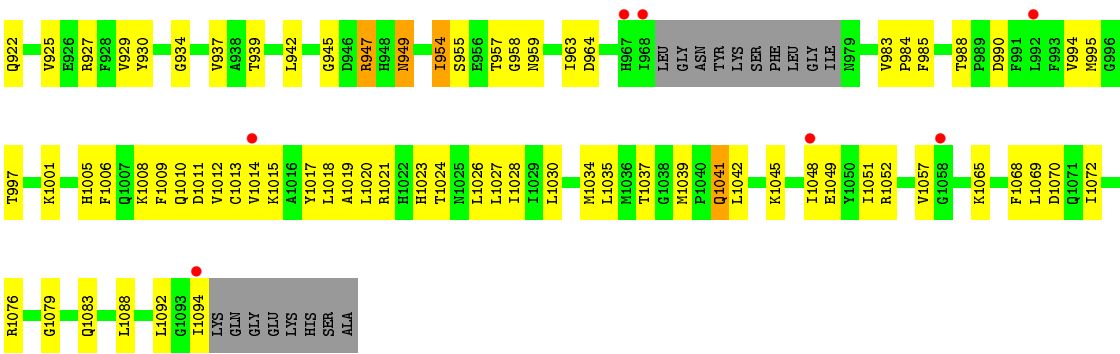
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total 135	O 135	0	0

### 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, $\alpha$ , $\beta$ , $\gamma$	142.83Å 67.33Å 106.26Å 90.00° 96.13° 90.00°	Depositor
Resolution (Å)	60.84 – 2.40 60.84 – 2.41	Depositor EDS
% Data completeness (in resolution range)	85.4 (60.84-2.40) 85.5 (60.84-2.41)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.273 , 0.309 0.258 , 0.297	Depositor DCC
$R_{free}$ test set	1630 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LY2

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	0.40	0/7035	0.57	0/9519

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6889	0	6962	305	0
2	A	23	0	17	2	0
3	A	135	0	0	38	0
All	All	7047	0	6979	305	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 (305) 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:579:ARG:HB3	1:A:610:LEU:HD11	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:LYS:HD2	1:A:1045:LYS:H	1.39	0.86
1:A:687:ARG:HG3	1:A:687:ARG:HH11	1.39	0.86
1:A:804:MET:HE3	1:A:810:PRO:HB2	1.59	0.85
1:A:654:ASP:HB3	3:A:2004:HOH:O	1.78	0.83
1:A:1088:LEU:HD23	1:A:1092:LEU:HD12	1.58	0.82
1:A:240:THR:HG22	1:A:242:GLY:H	1.47	0.79
1:A:689:LYS:HG2	1:A:728:MET:SD	2.24	0.78
1:A:843:LEU:HD23	1:A:1034:MET:HG3	1.66	0.76
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.67	0.76
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.68	0.76
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.49	0.75
1:A:1069:LEU:HD12	1:A:1072:ILE:HD12	1.69	0.74
1:A:385:ALA:C	1:A:386:ASN:HD22	1.91	0.74
1:A:880:GLU:O	2:A:3095:LY2:H162	1.87	0.74
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.69	0.73
1:A:154:LEU:O	1:A:158:ILE:HG12	1.89	0.73
1:A:611:LEU:O	1:A:614:ARG:HG3	1.90	0.72
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.04	0.72
1:A:1010:GLN:HB3	1:A:1069:LEU:HD11	1.72	0.72
1:A:947:ARG:HH11	1:A:947:ARG:HB3	1.55	0.72
1:A:683:LYS:HD3	1:A:687:ARG:HH22	1.54	0.71
1:A:739:ILE:O	1:A:743:GLN:HG2	1.90	0.70
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.73	0.70
1:A:1024:THR:O	1:A:1028:ILE:HG12	1.92	0.68
1:A:821:THR:HB	3:A:2105:HOH:O	1.93	0.67
1:A:182:THR:HB	1:A:183:PRO:HD3	1.78	0.66
1:A:561:THR:HB	1:A:591:LYS:NZ	2.10	0.65
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.32	0.65
1:A:660:LEU:HD11	1:A:695:LEU:HD12	1.78	0.64
1:A:815:PHE:HB2	3:A:2103:HOH:O	1.96	0.64
1:A:643:ILE:HG13	1:A:644:ALA:N	2.13	0.64
1:A:384:GLU:HG2	1:A:386:ASN:HD21	1.63	0.63
1:A:375:ARG:HG3	1:A:376:THR:H	1.63	0.63
1:A:319:ARG:HH12	1:A:320:LYS:HE2	1.64	0.62
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.80	0.62
1:A:990:ASP:O	1:A:994:VAL:HG23	1.99	0.62
1:A:640:VAL:O	1:A:643:ILE:HG12	1.99	0.62
1:A:681:LEU:HB3	1:A:695:LEU:HD11	1.80	0.61
1:A:738:VAL:HG21	1:A:783:PHE:CD1	2.35	0.61
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.82	0.61
1:A:841:ASP:O	1:A:845:LEU:HD22	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:O	1:A:287:ILE:HG23	2.01	0.61
1:A:737:GLN:O	1:A:741:MET:HG3	1.99	0.61
1:A:925:VAL:O	1:A:929:VAL:HG23	2.00	0.61
1:A:930:TYR:HA	3:A:2118:HOH:O	2.00	0.61
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.15	0.60
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.01	0.60
1:A:597:LYS:HD3	1:A:600:GLN:HE22	1.66	0.60
1:A:418:ILE:HG22	3:A:2046:HOH:O	2.01	0.60
1:A:559:ILE:HG23	1:A:588:ALA:HB2	1.84	0.60
1:A:428:LEU:HB3	3:A:2050:HOH:O	2.02	0.60
1:A:375:ARG:HG3	1:A:376:THR:N	2.17	0.59
1:A:844:ILE:O	1:A:848:LEU:HD13	2.02	0.59
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.17	0.59
1:A:662:GLN:HE21	1:A:1030:LEU:HD22	1.67	0.59
1:A:175:PHE:CZ	1:A:179:ARG:HD2	2.37	0.59
1:A:921:PHE:O	1:A:925:VAL:HG23	2.02	0.59
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.33	0.58
1:A:564:LEU:HD13	1:A:1049:GLU:HA	1.85	0.58
1:A:920:LYS:HA	3:A:2117:HOH:O	2.02	0.58
1:A:469:ILE:HG22	3:A:2054:HOH:O	2.02	0.58
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.32	0.58
1:A:180:LEU:O	1:A:183:PRO:HD2	2.03	0.58
1:A:742:LEU:HB3	3:A:2093:HOH:O	2.04	0.58
1:A:784:ARG:HG2	1:A:784:ARG:NH1	2.17	0.58
1:A:193:PRO:HB2	1:A:313:PRO:HB2	1.86	0.57
1:A:564:LEU:HD12	1:A:1052:ARG:HB2	1.86	0.57
1:A:597:LYS:HD3	1:A:600:GLN:NE2	2.20	0.57
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.85	0.57
1:A:954:ILE:HD13	1:A:955:SER:N	2.20	0.57
1:A:551:LEU:HD12	3:A:2066:HOH:O	2.04	0.57
1:A:860:LEU:HD21	1:A:1015:LYS:HE2	1.87	0.57
1:A:910:TRP:CZ2	1:A:914:LYS:HE3	2.40	0.56
1:A:405:THR:HG23	1:A:407:GLU:O	2.05	0.56
1:A:416:PHE:HB3	3:A:2046:HOH:O	2.04	0.56
1:A:387:ILE:HG22	1:A:394:LEU:HD12	1.87	0.56
1:A:784:ARG:HG2	1:A:784:ARG:HH11	1.69	0.56
1:A:364:LYS:HE3	1:A:411:ASN:HA	1.88	0.56
1:A:810:PRO:HG3	1:A:833:LYS:HG3	1.88	0.56
1:A:187:GLU:OE1	1:A:687:ARG:HG3	2.05	0.56
1:A:724:CYS:HB2	1:A:728:MET:CE	2.36	0.56
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HB	1:A:239:ASP:OD2	2.06	0.56
1:A:386:ASN:N	1:A:386:ASN:HD22	2.02	0.55
1:A:995:MET:O	1:A:1005:HIS:HB2	2.07	0.55
1:A:418:ILE:HD13	1:A:423:LEU:HD23	1.89	0.55
1:A:768:LYS:O	1:A:772:GLU:HG2	2.06	0.55
1:A:386:ASN:ND2	1:A:396:GLN:HG3	2.21	0.55
1:A:918:GLU:O	1:A:922:GLN:HG2	2.08	0.54
1:A:483:HIS:HD2	3:A:2058:HOH:O	1.90	0.54
1:A:184:ARG:NH1	1:A:722:ARG:HD3	2.23	0.54
1:A:187:GLU:HG2	1:A:686:LEU:HB2	1.88	0.54
1:A:425:LYS:HE2	3:A:2054:HOH:O	2.07	0.54
1:A:434:TYR:HA	1:A:459:GLN:O	2.06	0.54
1:A:568:THR:O	1:A:571:ASP:HB2	2.08	0.54
1:A:731:ASP:O	1:A:735:GLN:HG3	2.07	0.54
1:A:149:ALA:O	1:A:152:ARG:HB3	2.08	0.53
1:A:705:GLN:HG2	1:A:874:ASP:HA	1.90	0.53
1:A:218:ASN:O	1:A:236:SER:HA	2.09	0.53
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.38	0.53
1:A:568:THR:H	1:A:571:ASP:HB2	1.74	0.53
1:A:687:ARG:CG	1:A:687:ARG:HH11	2.16	0.53
1:A:743:GLN:HE22	1:A:876:ILE:CG2	2.21	0.53
1:A:389:TYR:O	1:A:392:GLN:HG2	2.09	0.53
1:A:419:LYS:HD2	1:A:421:LYS:HE2	1.91	0.53
1:A:519:LEU:HB2	3:A:2025:HOH:O	2.07	0.53
1:A:793:ALA:HB1	3:A:2097:HOH:O	2.09	0.53
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.39	0.52
1:A:983:VAL:HG23	1:A:984:PRO:HD2	1.92	0.52
1:A:828:ILE:HD12	3:A:2103:HOH:O	2.09	0.52
1:A:380:THR:HG22	3:A:2038:HOH:O	2.08	0.52
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.91	0.52
1:A:927:ARG:NH1	1:A:959:ASN:HD22	2.07	0.52
1:A:476:ARG:O	1:A:520:LEU:HD23	2.10	0.52
1:A:995:MET:CE	1:A:1009:PHE:HB2	2.40	0.52
1:A:469:ILE:HG13	3:A:2053:HOH:O	2.08	0.52
1:A:247:SER:O	1:A:251:LYS:HG2	2.10	0.51
1:A:995:MET:HE2	1:A:1009:PHE:HB2	1.92	0.51
1:A:549:ASN:O	1:A:552:ARG:HB3	2.10	0.51
1:A:561:THR:HB	1:A:591:LYS:HZ3	1.74	0.51
1:A:207:LEU:HD12	1:A:288:LYS:HD2	1.91	0.51
1:A:760:SER:O	1:A:763:VAL:HG12	2.10	0.51
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:ARG:NH1	1:A:959:ASN:ND2	2.59	0.51
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.76	0.51
1:A:368:ILE:HG21	1:A:433:ILE:CD1	2.40	0.51
1:A:889:ALA:O	1:A:893:GLN:HG3	2.11	0.51
1:A:927:ARG:HH11	1:A:959:ASN:ND2	2.08	0.51
1:A:1028:ILE:HD12	1:A:1051:ILE:HG23	1.92	0.51
1:A:240:THR:O	1:A:244:ILE:HG12	2.10	0.51
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.46	0.51
1:A:364:LYS:HZ1	1:A:411:ASN:C	2.14	0.51
1:A:357:CYS:HB2	3:A:2019:HOH:O	2.11	0.51
1:A:862:LEU:HB3	1:A:934:GLY:HA3	1.93	0.51
1:A:696:PHE:CE1	1:A:721:LEU:HD21	2.46	0.50
1:A:954:ILE:HA	1:A:959:ASN:O	2.11	0.50
1:A:475:LEU:HG	1:A:476:ARG:H	1.76	0.50
1:A:862:LEU:HD22	1:A:862:LEU:N	2.27	0.50
1:A:624:VAL:O	1:A:628:MET:HG2	2.12	0.50
1:A:477:HIS:HA	1:A:520:LEU:HB2	1.94	0.50
1:A:734:GLN:OE1	1:A:780:PRO:HB3	2.11	0.50
1:A:752:LEU:O	1:A:753:SER:HB3	2.12	0.50
1:A:937:VAL:HG23	3:A:2119:HOH:O	2.11	0.50
1:A:660:LEU:O	1:A:664:VAL:HG23	2.12	0.50
1:A:361:PHE:HA	3:A:2062:HOH:O	2.11	0.50
1:A:792:LYS:HB3	1:A:818:ALA:HB3	1.93	0.50
1:A:743:GLN:HE22	1:A:876:ILE:HG21	1.75	0.49
1:A:384:GLU:HG2	1:A:386:ASN:ND2	2.26	0.49
1:A:687:ARG:NH1	1:A:687:ARG:HG3	2.17	0.49
1:A:1041:GLN:H	1:A:1041:GLN:NE2	2.11	0.49
1:A:209:GLU:HB3	1:A:859:SER:HB3	1.94	0.49
1:A:888:ILE:HD11	1:A:954:ILE:HB	1.94	0.49
1:A:176:THR:O	1:A:180:LEU:HG	2.12	0.49
1:A:929:VAL:HG13	1:A:995:MET:CE	2.42	0.49
1:A:1023:HIS:HA	3:A:2128:HOH:O	2.12	0.49
1:A:477:HIS:HA	1:A:520:LEU:CB	2.42	0.49
1:A:170:ASP:OD1	1:A:172:GLU:HB2	2.13	0.49
1:A:808:LYS:HB3	1:A:834:HIS:O	2.12	0.49
1:A:364:LYS:HB2	1:A:413:TRP:CD2	2.48	0.49
1:A:158:ILE:HG22	1:A:703:ILE:HD13	1.95	0.49
1:A:644:ALA:HA	3:A:2072:HOH:O	2.13	0.48
1:A:576:TRP:O	1:A:579:ARG:HG3	2.13	0.48
1:A:551:LEU:HA	3:A:2066:HOH:O	2.12	0.48
1:A:597:LYS:HB2	1:A:603:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ASP:O	1:A:575:LEU:HB2	2.14	0.48
1:A:1008:LYS:O	1:A:1012:VAL:HG23	2.14	0.48
1:A:1088:LEU:HB3	1:A:1094:ILE:HD12	1.95	0.48
1:A:245:LEU:HD21	1:A:272:LEU:HG	1.95	0.48
1:A:744:LYS:HB3	3:A:2092:HOH:O	2.13	0.48
1:A:858:GLU:OE1	1:A:1019:ALA:HA	2.14	0.48
1:A:681:LEU:HA	3:A:2083:HOH:O	2.14	0.48
1:A:760:SER:O	1:A:764:ILE:HG13	2.14	0.48
1:A:362:ARG:HB3	1:A:415:GLU:HA	1.95	0.47
1:A:558:ILE:HG22	3:A:2069:HOH:O	2.12	0.47
1:A:720:TYR:OH	1:A:728:MET:HE3	2.14	0.47
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.14	0.47
1:A:732:PHE:O	1:A:736:VAL:HG23	2.14	0.47
1:A:796:LEU:HG	1:A:815:PHE:CE2	2.49	0.47
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.96	0.47
1:A:1024:THR:HG21	1:A:1057:VAL:HG22	1.96	0.47
1:A:464:VAL:HG21	1:A:482:LEU:HB3	1.96	0.47
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.49	0.47
1:A:1006:PHE:O	1:A:1009:PHE:HB3	2.15	0.47
1:A:430:ASN:OD1	1:A:432:GLN:HG3	2.15	0.47
1:A:743:GLN:HA	1:A:743:GLN:HE21	1.80	0.46
1:A:366:ARG:HG2	3:A:2021:HOH:O	2.14	0.46
1:A:366:ARG:NH1	3:A:2028:HOH:O	2.48	0.46
1:A:460:LEU:HG	1:A:487:LEU:HD12	1.98	0.46
1:A:769:GLN:O	1:A:772:GLU:HB2	2.15	0.46
1:A:997:THR:HG21	1:A:1076:ARG:HH21	1.81	0.46
1:A:887:THR:HG23	1:A:890:LYS:HB2	1.96	0.46
1:A:827:THR:O	1:A:883:LYS:HE2	2.16	0.46
1:A:649:GLU:HA	1:A:680:PHE:HE1	1.79	0.46
1:A:851:MET:HG2	1:A:1020:LEU:HD21	1.98	0.46
1:A:199:HIS:HB3	1:A:689:LYS:HB2	1.98	0.46
1:A:895:THR:CG2	1:A:906:VAL:HG22	2.47	0.45
1:A:1011:ASP:O	1:A:1015:LYS:HB2	2.16	0.45
1:A:163:THR:O	1:A:165:VAL:HG13	2.17	0.45
1:A:498:ASN:ND2	1:A:1042:LEU:HD23	2.31	0.45
1:A:554:GLN:HA	1:A:554:GLN:NE2	2.31	0.45
1:A:362:ARG:CB	1:A:415:GLU:HA	2.46	0.45
1:A:462:TYR:CE1	1:A:486:GLN:HG3	2.52	0.45
1:A:576:TRP:O	1:A:577:HIS:C	2.54	0.45
1:A:833:LYS:O	1:A:876:ILE:HG13	2.17	0.45
1:A:206:PRO:O	1:A:208:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:TYR:HB2	1:A:590:PRO:HD3	1.97	0.45
1:A:758:ASP:O	1:A:760:SER:N	2.50	0.45
1:A:954:ILE:HD11	1:A:958:GLY:HA2	1.97	0.45
1:A:997:THR:HG23	1:A:1001:LYS:O	2.17	0.45
1:A:210:TYR:OH	1:A:856:GLU:HG3	2.17	0.45
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.17	0.44
1:A:184:ARG:HH12	1:A:722:ARG:HD3	1.83	0.44
1:A:150:PHE:O	1:A:153:GLN:HG2	2.18	0.44
1:A:855:TRP:CE3	1:A:862:LEU:HD23	2.52	0.44
1:A:393:VAL:O	1:A:393:VAL:HG23	2.17	0.44
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.98	0.44
1:A:358:ASP:OD1	1:A:421:LYS:HD3	2.17	0.44
1:A:567:LEU:HD11	1:A:591:LYS:HD2	1.99	0.44
1:A:1039:MET:HB3	1:A:1041:GLN:OE1	2.17	0.44
1:A:273:ARG:HD3	1:A:280:TYR:CE2	2.53	0.44
1:A:354:LEU:HA	1:A:527:ILE:O	2.17	0.44
1:A:312:ASP:C	1:A:314:ALA:H	2.20	0.44
1:A:241:PRO:O	1:A:245:LEU:HG	2.18	0.44
1:A:379:LEU:HB2	1:A:404:PHE:HB3	1.99	0.43
1:A:840:GLN:O	1:A:844:ILE:HG12	2.18	0.43
1:A:771:LEU:HA	1:A:774:LEU:HD12	2.00	0.43
1:A:887:THR:HG22	2:A:3095:LY2:H22	2.00	0.43
1:A:376:THR:HG22	3:A:2036:HOH:O	2.18	0.43
1:A:425:LYS:HG3	3:A:2054:HOH:O	2.18	0.43
1:A:607:THR:O	1:A:610:LEU:HB2	2.19	0.43
1:A:988:THR:HG21	1:A:1083:GLN:HG3	2.00	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.18	0.43
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.48	0.43
1:A:687:ARG:NH1	1:A:687:ARG:CG	2.79	0.43
1:A:725:GLY:O	1:A:729:LEU:HB2	2.18	0.43
1:A:910:TRP:O	1:A:914:LYS:HG2	2.18	0.43
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.53	0.43
1:A:796:LEU:HD23	1:A:814:GLU:O	2.19	0.43
1:A:743:GLN:NE2	1:A:876:ILE:HG21	2.34	0.43
1:A:479:GLU:HG2	3:A:2025:HOH:O	2.18	0.43
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.95	0.43
1:A:696:PHE:CD1	1:A:721:LEU:HD21	2.54	0.43
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.84	0.43
1:A:843:LEU:CD2	1:A:1034:MET:HG3	2.45	0.43
1:A:1035:LEU:HA	1:A:1039:MET:HG2	2.01	0.42
1:A:390:GLY:O	1:A:391:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:LYS:CB	1:A:906:VAL:HG23	2.44	0.42
1:A:364:LYS:HE2	1:A:411:ASN:OD1	2.20	0.42
1:A:499:ALA:HB2	1:A:1037:THR:HG22	2.01	0.42
1:A:586:PRO:C	1:A:588:ALA:H	2.22	0.42
1:A:784:ARG:CG	1:A:784:ARG:HH11	2.32	0.42
1:A:574:LEU:HD23	1:A:574:LEU:C	2.39	0.42
1:A:770:LYS:O	1:A:774:LEU:HG	2.18	0.42
1:A:949:ASN:HD22	1:A:949:ASN:HA	1.68	0.42
1:A:380:THR:O	1:A:435:CYS:HA	2.19	0.42
1:A:682:LEU:HD22	1:A:686:LEU:CD1	2.50	0.42
1:A:947:ARG:NH1	1:A:947:ARG:HB3	2.29	0.42
1:A:379:LEU:O	1:A:403:PRO:HA	2.20	0.42
1:A:845:LEU:O	1:A:848:LEU:HB2	2.20	0.42
1:A:309:THR:HA	1:A:310:PRO:HD3	1.93	0.42
1:A:905:GLU:CD	1:A:905:GLU:H	2.20	0.42
1:A:147:THR:HG23	1:A:319:ARG:HH21	1.84	0.42
1:A:568:THR:N	1:A:571:ASP:HB2	2.34	0.42
1:A:559:ILE:CG2	1:A:588:ALA:HB2	2.50	0.42
1:A:837:ASP:OD1	1:A:839:ARG:HB2	2.20	0.42
1:A:862:LEU:CD2	1:A:862:LEU:N	2.83	0.42
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.20	0.42
1:A:984:PRO:HG2	1:A:985:PHE:H	1.85	0.42
1:A:466:LEU:HA	3:A:2051:HOH:O	2.20	0.41
1:A:470:ASP:OD2	1:A:474:LEU:HB2	2.20	0.41
1:A:520:LEU:O	1:A:521:ASP:C	2.58	0.41
1:A:798:ILE:HG13	1:A:798:ILE:H	1.65	0.41
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.20	0.41
1:A:240:THR:HG23	1:A:241:PRO:HD2	2.01	0.41
1:A:816:LYS:HE3	3:A:2098:HOH:O	2.20	0.41
1:A:833:LYS:HE3	1:A:836:ASP:HB2	2.01	0.41
1:A:518:ILE:HD12	1:A:520:LEU:CD1	2.51	0.41
1:A:584:LYS:HA	1:A:616:VAL:HG11	2.02	0.41
1:A:180:LEU:C	1:A:183:PRO:HD2	2.41	0.41
1:A:290:PHE:HB2	1:A:293:VAL:HG23	2.03	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.21	0.41
1:A:867:TYR:OH	1:A:963:ILE:HA	2.21	0.41
1:A:422:ASP:HB3	1:A:599:GLY:O	2.20	0.41
1:A:170:ASP:OD1	1:A:172:GLU:N	2.53	0.41
1:A:182:THR:HG22	3:A:2003:HOH:O	2.21	0.41
1:A:910:TRP:CE2	1:A:914:LYS:HE3	2.55	0.41
1:A:519:LEU:HD21	3:A:2034:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ARG:O	1:A:645:VAL:HG23	2.21	0.41
1:A:462:TYR:HA	1:A:485:TRP:O	2.21	0.41
1:A:506:THR:HB	3:A:2057:HOH:O	2.21	0.41
1:A:749:ILE:HG13	1:A:767:LEU:HD23	2.03	0.41
1:A:915:CYS:HA	1:A:916:PRO:HD2	1.96	0.41
1:A:744:LYS:HG2	1:A:748:ASP:OD1	2.20	0.40
1:A:791:LEU:HD13	1:A:828:ILE:HD13	2.03	0.40
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.51	0.40
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.35	0.40
1:A:374:PRO:HB3	3:A:2036:HOH:O	2.20	0.40
1:A:689:LYS:HE2	1:A:728:MET:CG	2.52	0.40
1:A:364:LYS:CE	1:A:411:ASN:OD1	2.69	0.40
1:A:386:ASN:HD21	1:A:396:GLN:HG3	1.85	0.40
1:A:480:TYR:HB2	1:A:518:ILE:HG12	2.03	0.40
1:A:712:ARG:O	1:A:716:ILE:HG13	2.22	0.40
1:A:895:THR:HG21	1:A:906:VAL:HG22	2.02	0.40
1:A:929:VAL:HA	1:A:995:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	836/961 (87%)	743 (89%)	81 (10%)	12 (1%)	11	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	VAL
1	A	144	SER
1	A	521	ASP
1	A	524	CYS

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Mol	Chain	Res	Type
1	A	587	LYS
1	A	859	SER
1	A	509	ASP
1	A	549	ASN
1	A	964	ASP
1	A	208	PRO
1	A	753	SER
1	A	1079	GLY

### 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	766/857 (89%)	722 (94%)	44 (6%)	20	33

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	VAL
1	A	207	LEU
1	A	218	ASN
1	A	285	THR
1	A	369	ASP
1	A	395	CYS
1	A	410	TRP
1	A	471	HIS
1	A	522	ASN
1	A	579	ARG
1	A	601	GLN
1	A	616	VAL
1	A	626	LEU
1	A	682	LEU
1	A	687	ARG
1	A	690	ARG
1	A	695	LEU
1	A	706	SER

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Mol	Chain	Res	Type
1	A	717	LEU
1	A	728	MET
1	A	743	GLN
1	A	757	TYR
1	A	775	GLN
1	A	778	ASN
1	A	781	GLN
1	A	799	GLU
1	A	841	ASP
1	A	845	LEU
1	A	847	ILE
1	A	876	ILE
1	A	883	LYS
1	A	887	THR
1	A	899	THR
1	A	905	GLU
1	A	907	LEU
1	A	915	CYS
1	A	947	ARG
1	A	949	ASN
1	A	954	ILE
1	A	957	THR
1	A	1026	LEU
1	A	1027	LEU
1	A	1041	GLN
1	A	1070	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	299	ASN
1	A	304	HIS
1	A	386	ASN
1	A	396	GLN
1	A	459	GLN
1	A	483	HIS
1	A	522	ASN
1	A	550	GLN
1	A	554	GLN
1	A	565	ASN
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	609	GLN
1	A	662	GLN
1	A	705	GLN
1	A	710	GLN
1	A	730	HIS
1	A	743	GLN
1	A	949	ASN
1	A	951	ASN
1	A	959	ASN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	LY2	A	3095	-	23,26,26	3.03	13 (56%)	28,36,36	1.27	4 (14%)

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	LY2	A	3095	-	-	5/6/16/16	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3095	LY2	C10-C9	8.05	1.53	1.37
2	A	3095	LY2	O12-C11	5.33	1.42	1.35
2	A	3095	LY2	C5-C20	-4.01	1.42	1.49
2	A	3095	LY2	O12-C4	4.00	1.43	1.36
2	A	3095	LY2	C6-C5	3.48	1.44	1.38
2	A	3095	LY2	C11-N14	3.09	1.46	1.36
2	A	3095	LY2	C3-C4	3.01	1.45	1.41
2	A	3095	LY2	C25-C20	2.82	1.45	1.39
2	A	3095	LY2	C21-C20	2.73	1.45	1.39
2	A	3095	LY2	C19-N14	2.68	1.50	1.46
2	A	3095	LY2	C15-N14	2.64	1.50	1.46
2	A	3095	LY2	C1-C2	2.44	1.42	1.36
2	A	3095	LY2	C24-C25	2.12	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3095	LY2	C10-C9-C3	-3.63	119.03	123.05
2	A	3095	LY2	C2-C3-C4	2.58	119.49	116.50
2	A	3095	LY2	O12-C4-C3	-2.30	118.98	121.20
2	A	3095	LY2	C18-O17-C16	2.01	116.59	109.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

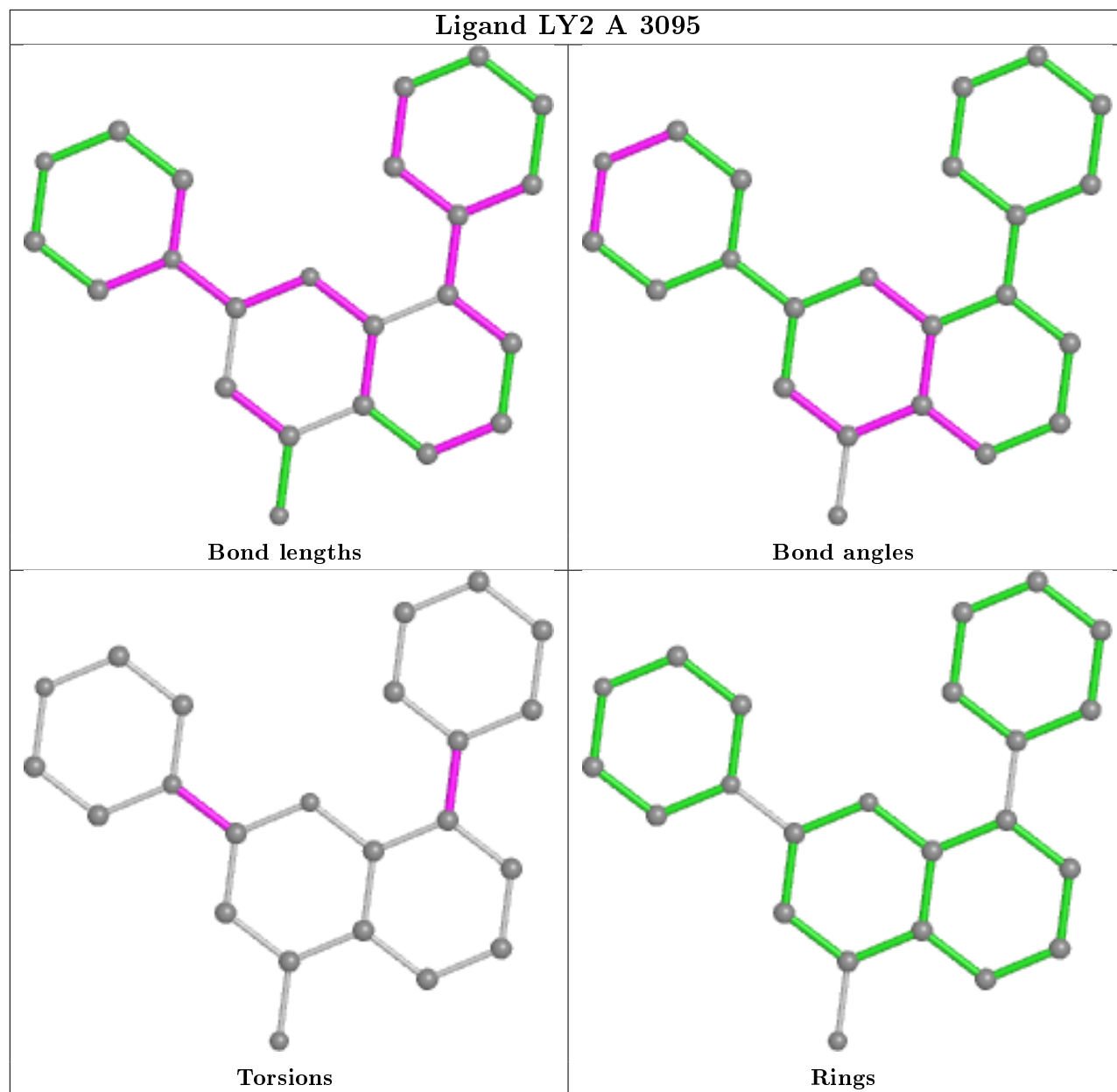
Mol	Chain	Res	Type	Atoms
2	A	3095	LY2	C10-C11-N14-C19
2	A	3095	LY2	C21-C20-C5-C4
2	A	3095	LY2	C25-C20-C5-C4
2	A	3095	LY2	C25-C20-C5-C6
2	A	3095	LY2	C21-C20-C5-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3095	LY2	2	0

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, 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	850/961 (88%)	0.63	69 (8%) 12 11	31, 75, 117, 132	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	PHE	5.4
1	A	522	ASN	5.3
1	A	564	LEU	4.7
1	A	529	LEU	4.7
1	A	524	CYS	4.3
1	A	359	ARG	3.8
1	A	967	HIS	3.8
1	A	823	LEU	3.7
1	A	749	ILE	3.6
1	A	221	PHE	3.4
1	A	523	TYR	3.4
1	A	231	GLN	3.4
1	A	410	TRP	3.4
1	A	211	LEU	3.3
1	A	527	ILE	3.2
1	A	767	LEU	3.2
1	A	559	ILE	3.1
1	A	355	TRP	3.1
1	A	237	ALA	3.0
1	A	968	ILE	2.9
1	A	553	LYS	2.9
1	A	408	VAL	2.9
1	A	419	LYS	2.8
1	A	413	TRP	2.8
1	A	428	LEU	2.8
1	A	755	GLU	2.8
1	A	358	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	248	PHE	2.8
1	A	461	LEU	2.8
1	A	771	LEU	2.7
1	A	356	ASP	2.7
1	A	368	ILE	2.7
1	A	757	TYR	2.6
1	A	409	LEU	2.6
1	A	1094	ILE	2.6
1	A	899	THR	2.6
1	A	768	LYS	2.6
1	A	307	LEU	2.5
1	A	487	LEU	2.5
1	A	412	VAL	2.5
1	A	1048	ILE	2.5
1	A	822	ALA	2.4
1	A	235	VAL	2.4
1	A	555	LEU	2.4
1	A	901	ALA	2.4
1	A	162	VAL	2.4
1	A	1058	GLY	2.3
1	A	992	LEU	2.3
1	A	165	VAL	2.3
1	A	387	ILE	2.3
1	A	287	ILE	2.3
1	A	212	LEU	2.3
1	A	421	LYS	2.2
1	A	306	VAL	2.1
1	A	919	GLU	2.1
1	A	520	LEU	2.1
1	A	233	ILE	2.1
1	A	370	ILE	2.1
1	A	354	LEU	2.1
1	A	379	LEU	2.1
1	A	383	VAL	2.1
1	A	1014	VAL	2.1
1	A	546	GLU	2.0
1	A	582	SER	2.0
1	A	249	PHE	2.0
1	A	226	ARG	2.0
1	A	563	PRO	2.0
1	A	272	LEU	2.0
1	A	578	PHE	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](#)

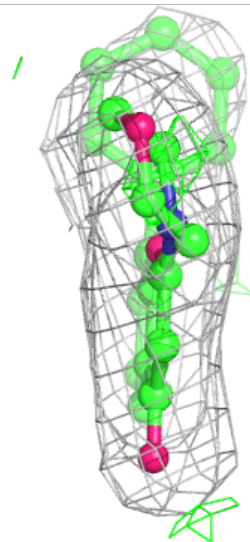
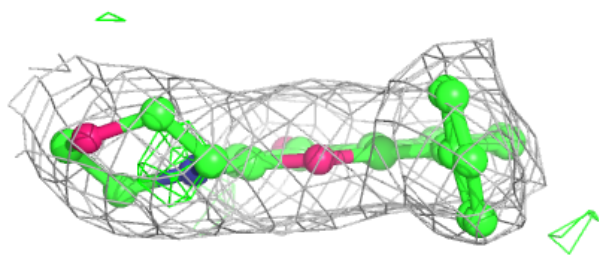
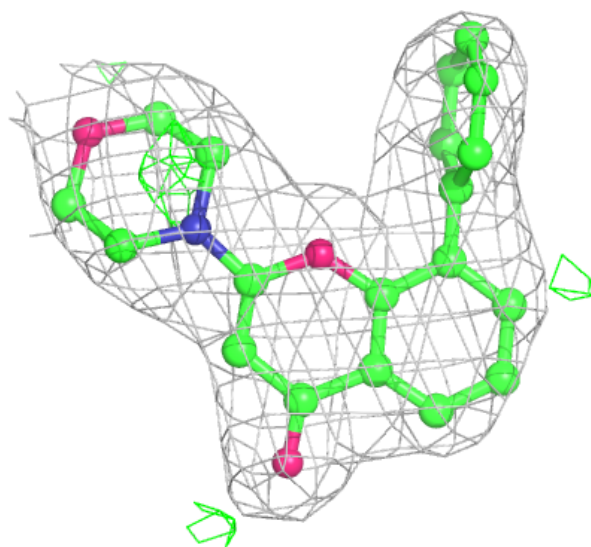
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LY2	A	3095	23/23	0.93	0.19	50,55,65,67	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.

**Electron density around LY2 A 3095:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.