



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:08 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

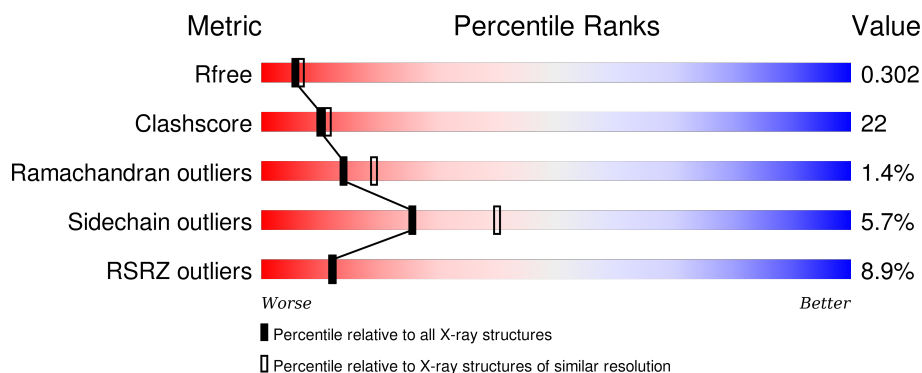
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	

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.

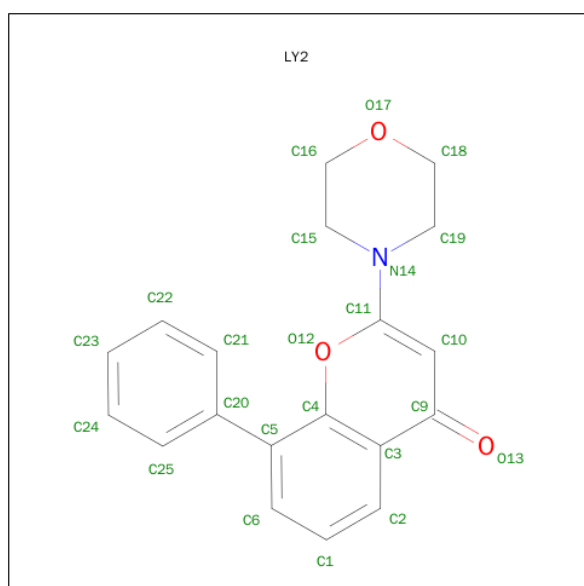
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

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

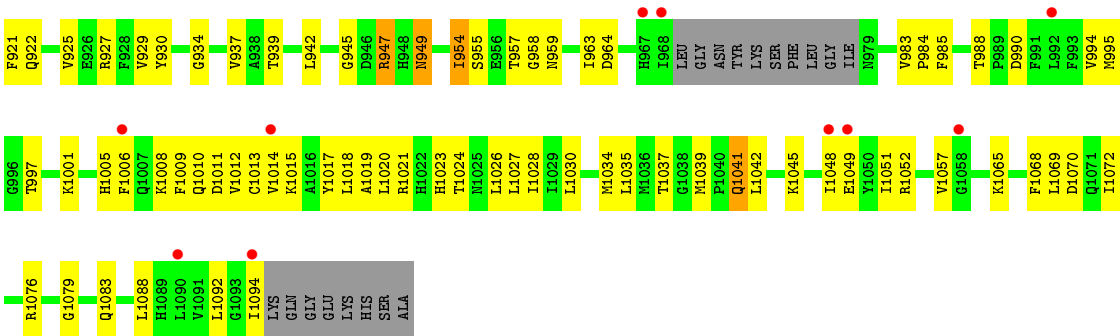
- Molecule 2 is 2-MORPHOLIN-4-YL-7-PHENYL-4H-CHROMEN-4-ONE (three-letter code: LY2) (formula: C₁₉H₁₇NO₃).



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.83 Å 67.33 Å 106.26 Å 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
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.40 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.273 , 0.309 0.268 , 0.302	Depositor DCC
R_{free} test set	1630 reflections (4.86%)	DCC
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33524 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Continued on next page...

Continued from previous page...

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:HH11	1:A:687:ARG:HG3	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:990:ASP:O	1:A:994:VAL:HG23	1.99	0.62
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.80	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:841:ASP:O	1:A:845:LEU:HD22	1.98	0.61
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.82	0.61

Continued on next page...

Continued from previous page...

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:597:LYS:HD3	1:A:600:GLN:HE22	1.66	0.60
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.01	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:784:ARG:HG2	1:A:784:ARG:NH1	2.17	0.58
1:A:742:LEU:HB3	3:A:2093:HOH:O	2.04	0.58
1:A:193:PRO:HB2	1:A:313:PRO:HB2	1.86	0.57
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.85	0.57
1:A:597:LYS:HD3	1:A:600:GLN:NE2	2.20	0.57
1:A:564:LEU:HD12	1:A:1052:ARG:HB2	1.86	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:416:PHE:HB3	3:A:2046:HOH:O	2.04	0.56
1:A:405:THR:HG23	1:A:407:GLU:O	2.05	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

Continued on next page...

Continued from previous page...

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:903:LYS:HB2	1:A:906:VAL:CG2	2.38	0.53
1:A:218:ASN:O	1:A:236:SER:HA	2.09	0.53
1:A:687:ARG:HH11	1:A:687:ARG:CG	2.16	0.53
1:A:743:GLN:HE22	1:A:876:ILE:CG2	2.21	0.53
1:A:568:THR:H	1:A:571:ASP:HB2	1.74	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:793:ALA:HB1	3:A:2097:HOH:O	2.09	0.53
1:A:519:LEU:HB2	3:A:2025:HOH:O	2.07	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: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:380:THR:HG22	3:A:2038:HOH:O	2.08	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:561:THR:HB	1:A:591:LYS:HZ3	1.74	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:760:SER:O	1:A:763:VAL:HG12	2.10	0.51
1:A:207:LEU:HD12	1:A:288:LYS:HD2	1.91	0.51
1:A:927:ARG:NH1	1:A:959:ASN:ND2	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.91	0.51
1:A:368:ILE:HG21	1:A:433:ILE:CD1	2.40	0.51
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.76	0.51
1:A:927:ARG:HH11	1:A:959:ASN:ND2	2.08	0.51
1:A:889:ALA:O	1:A:893:GLN:HG3	2.11	0.51
1:A:240:THR:O	1:A:244:ILE:HG12	2.10	0.51
1:A:1028:ILE:HD12	1:A:1051:ILE:HG23	1.92	0.51
1:A:364:LYS:HZ1	1:A:411:ASN:C	2.14	0.51
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.46	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:954:ILE:HA	1:A:959:ASN:O	2.11	0.50
1:A:696:PHE:CE1	1:A:721:LEU:HD21	2.46	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:937:VAL:HG23	3:A:2119:HOH:O	2.11	0.50
1:A:752:LEU:O	1:A:753:SER:HB3	2.12	0.50
1:A:734:GLN:OE1	1:A:780:PRO:HB3	2.11	0.50
1:A:660:LEU:O	1:A:664:VAL:HG23	2.12	0.50
1:A:792:LYS:HB3	1:A:818:ALA:HB3	1.93	0.50
1:A:361:PHE:HA	3:A:2062:HOH:O	2.11	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:477:HIS:HA	1:A:520:LEU:CB	2.42	0.49
1:A:1023:HIS:HA	3:A:2128:HOH:O	2.12	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:158:ILE:HG22	1:A:703:ILE:HD13	1.95	0.49
1:A:364:LYS:HB2	1:A:413:TRP:CD2	2.48	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:597:LYS:HB2	1:A:603:ILE:CD1	2.44	0.48
1:A:551:LEU:HA	3:A:2066:HOH:O	2.12	0.48

Continued on next page...

Continued from previous page...

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: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:1008:LYS:O	1:A:1012:VAL:HG23	2.14	0.48
1:A:681:LEU:HA	3:A:2083:HOH:O	2.14	0.48
1:A:858:GLU:OE1	1:A:1019:ALA:HA	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:720:TYR:OH	1:A:728:MET:HE3	2.14	0.47
1:A:558:ILE:HG22	3:A:2069:HOH:O	2.12	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:430:ASN:OD1	1:A:432:GLN:HG3	2.15	0.47
1:A:1006:PHE:O	1:A:1009:PHE:HB3	2.15	0.47
1:A:743:GLN:HA	1:A:743:GLN:HE21	1.80	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: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: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:954:ILE:HD11	1:A:958:GLY:HA2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ASP:O	1:A:760:SER:N	2.50	0.45
1:A:589:TYR:HB2	1:A:590:PRO:HD3	1.97	0.45
1:A:206:PRO:O	1:A:208:PRO:HD3	2.17	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:855:TRP:CE3	1:A:862:LEU:HD23	2.52	0.44
1:A:150:PHE:O	1:A:153:GLN:HG2	2.18	0.44
1:A:393:VAL:O	1:A:393:VAL:HG23	2.17	0.44
1:A:567:LEU:HD11	1:A:591:LYS:HD2	1.99	0.44
1:A:358:ASP:OD1	1:A:421:LYS:HD3	2.17	0.44
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.98	0.44
1:A:1039:MET:HB3	1:A:1041:GLN:OE1	2.17	0.44
1:A:354:LEU:HA	1:A:527:ILE:O	2.17	0.44
1:A:273:ARG:HD3	1:A:280:TYR:CE2	2.53	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:887:THR:HG22	2:A:3095:LY2:H22	2.00	0.43
1:A:771:LEU:HA	1:A:774:LEU:HD12	2.00	0.43
1:A:607:THR:O	1:A:610:LEU:HB2	2.19	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:988:THR:HG21	1:A:1083:GLN:HG3	2.00	0.43
1:A:687:ARG:NH1	1:A:687:ARG:CG	2.79	0.43
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.48	0.43
1:A:910:TRP:O	1:A:914:LYS:HG2	2.18	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.18	0.43
1:A:725:GLY:O	1:A:729:LEU:HB2	2.18	0.43
1:A:743:GLN:NE2	1:A:876:ILE:HG21	2.34	0.43
1:A:796:LEU:HD23	1:A:814:GLU:O	2.19	0.43
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.53	0.43
1:A:479:GLU:HG2	3:A:2025:HOH:O	2.18	0.43
1:A:696:PHE:CD1	1:A:721:LEU:HD21	2.54	0.43
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.95	0.43
1:A:843:LEU:CD2	1:A:1034:MET:HG3	2.45	0.43
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.84	0.43
1:A:903:LYS:CB	1:A:906:VAL:HG23	2.44	0.42
1:A:1035:LEU:HA	1:A:1039:MET:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLY:O	1:A:391:GLN:HB3	2.19	0.42
1:A:586:PRO:C	1:A:588:ALA:H	2.22	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:784:ARG:CG	1:A:784:ARG:HH11	2.32	0.42
1:A:770:LYS:O	1:A:774:LEU:HG	2.18	0.42
1:A:574:LEU:HD23	1:A:574:LEU:C	2.39	0.42
1:A:949:ASN:HD22	1:A:949:ASN:HA	1.68	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:380:THR:O	1:A:435:CYS:HA	2.19	0.42
1:A:845:LEU:O	1:A:848:LEU:HB2	2.20	0.42
1:A:379:LEU:O	1:A:403:PRO:HA	2.20	0.42
1:A:905:GLU:CD	1:A:905:GLU:H	2.20	0.42
1:A:309:THR:HA	1:A:310:PRO:HD3	1.93	0.42
1:A:147:THR:HG23	1:A:319:ARG:HH21	1.84	0.42
1:A:559:ILE:CG2	1:A:588:ALA:HB2	2.50	0.42
1:A:568:THR:N	1:A:571:ASP:HB2	2.34	0.42
1:A:837:ASP:OD1	1:A:839:ARG:HB2	2.20	0.42
1:A:984:PRO:HG2	1:A:985:PHE:H	1.85	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: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:466:LEU:HA	3:A:2051:HOH:O	2.20	0.41
1:A:833:LYS:HE3	1:A:836:ASP:HB2	2.01	0.41
1:A:240:THR:HG23	1:A:241:PRO:HD2	2.01	0.41
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.20	0.41
1:A:816:LYS:HE3	3:A:2098:HOH:O	2.20	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:867:TYR:OH	1:A:963:ILE:HA	2.21	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:422:ASP:HB3	1:A:599:GLY:O	2.20	0.41
1:A:182:THR:HG22	3:A:2003:HOH:O	2.21	0.41
1:A:170:ASP:OD1	1:A:172:GLU:N	2.53	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:TYR:HA	1:A:485:TRP:O	2.21	0.41
1:A:641:ARG:O	1:A:645:VAL:HG23	2.21	0.41
1:A:749:ILE:HG13	1:A:767:LEU:HD23	2.03	0.41
1:A:506:THR:HB	3:A:2057:HOH:O	2.21	0.41
1:A:915:CYS:HA	1:A:916:PRO:HD2	1.96	0.41
1:A:791:LEU:HD13	1:A:828:ILE:HD13	2.03	0.40
1:A:744:LYS:HG2	1:A:748:ASP:OD1	2.20	0.40
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.51	0.40
1:A:689:LYS:HE2	1:A:728:MET:CG	2.52	0.40
1:A:374:PRO:HB3	3:A:2036:HOH:O	2.20	0.40
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.35	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:364:LYS:CE	1:A:411:ASN:OD1	2.69	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 [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	836/961 (87%)	743 (89%)	81 (10%)	12 (1%)	14 19

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

Continued on next page...

Continued from previous page...

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%)	25	40

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	3.68	14 (60%)	28,36,36	1.05	1 (3%)

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	-	-	0/6/16/16	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3095	LY2	C5-C20	-3.93	1.42	1.49
2	A	3095	LY2	C24-C25	2.18	1.43	1.38
2	A	3095	LY2	C1-C2	2.44	1.42	1.36
2	A	3095	LY2	C21-C20	2.73	1.45	1.39
2	A	3095	LY2	C15-N14	2.73	1.50	1.46
2	A	3095	LY2	C19-N14	2.77	1.50	1.46
2	A	3095	LY2	C25-C20	2.82	1.45	1.39
2	A	3095	LY2	C11-N14	3.08	1.46	1.36
2	A	3095	LY2	C3-C4	3.26	1.45	1.41
2	A	3095	LY2	C6-C5	3.59	1.44	1.38
2	A	3095	LY2	O12-C4	3.63	1.43	1.36
2	A	3095	LY2	O12-C11	5.76	1.42	1.35
2	A	3095	LY2	C10-C9	7.84	1.53	1.37
2	A	3095	LY2	C9-C3	9.91	1.55	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3095	LY2	O12-C4-C3	-2.11	118.98	121.21

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	850/961 (88%)	0.70	76 (8%) 12 12	31, 75, 117, 132	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	PHE	5.5
1	A	522	ASN	5.5
1	A	564	LEU	4.9
1	A	529	LEU	4.9
1	A	524	CYS	4.5
1	A	359	ARG	4.0
1	A	967	HIS	3.9
1	A	823	LEU	3.8
1	A	749	ILE	3.7
1	A	221	PHE	3.5
1	A	231	GLN	3.5
1	A	523	TYR	3.5
1	A	410	TRP	3.5
1	A	211	LEU	3.4
1	A	527	ILE	3.4
1	A	767	LEU	3.3
1	A	559	ILE	3.3
1	A	355	TRP	3.2
1	A	237	ALA	3.2
1	A	968	ILE	3.1
1	A	408	VAL	3.0
1	A	553	LYS	3.0
1	A	413	TRP	3.0
1	A	419	LYS	3.0
1	A	428	LEU	2.9
1	A	358	ASP	2.9
1	A	755	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	461	LEU	2.9
1	A	356	ASP	2.9
1	A	771	LEU	2.9
1	A	248	PHE	2.9
1	A	368	ILE	2.8
1	A	1094	ILE	2.8
1	A	757	TYR	2.8
1	A	409	LEU	2.7
1	A	899	THR	2.7
1	A	307	LEU	2.7
1	A	487	LEU	2.7
1	A	768	LYS	2.7
1	A	412	VAL	2.7
1	A	1048	ILE	2.6
1	A	822	ALA	2.6
1	A	235	VAL	2.6
1	A	162	VAL	2.5
1	A	555	LEU	2.5
1	A	901	ALA	2.5
1	A	1058	GLY	2.5
1	A	165	VAL	2.5
1	A	992	LEU	2.4
1	A	387	ILE	2.4
1	A	287	ILE	2.4
1	A	212	LEU	2.4
1	A	421	LYS	2.3
1	A	306	VAL	2.3
1	A	1014	VAL	2.3
1	A	354	LEU	2.2
1	A	520	LEU	2.2
1	A	383	VAL	2.2
1	A	919	GLU	2.2
1	A	233	ILE	2.2
1	A	370	ILE	2.2
1	A	379	LEU	2.2
1	A	563	PRO	2.2
1	A	582	SER	2.1
1	A	546	GLU	2.1
1	A	226	ARG	2.1
1	A	249	PHE	2.1
1	A	272	LEU	2.1
1	A	369	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	896	VAL	2.1
1	A	578	PHE	2.1
1	A	1006	PHE	2.1
1	A	1090	LEU	2.1
1	A	210	TYR	2.1
1	A	551	LEU	2.0
1	A	1049	GLU	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	LY2	A	3095	23/23	0.93	0.19	0.04	50,55,65,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.