



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 AM GMT

PDB ID : 2CHZ  
Title : A PHARMACOLOGICAL MAP OF THE PI3-K FAMILY DEFINES A ROLE FOR P110ALPHA IN SIGNALING: THE STRUCTURE OF COMPLEX OF PHOSPHOINOSITIDE 3-KINASE GAMMA WITH INHIBITOR PIK-93  
Authors : Knight, Z.A.; Gonzalez, B.; Feldman, M.E.; Zunder, E.R.; Goldenberg, D.D.; Williams, O.; Loewith, R.; Stokoe, D.; Balla, A.; Toth, B.; Balla, T.; Weiss, W.A.; Williams, R.L.; Shokat, K.M.  
Deposited on : 2006-03-16  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

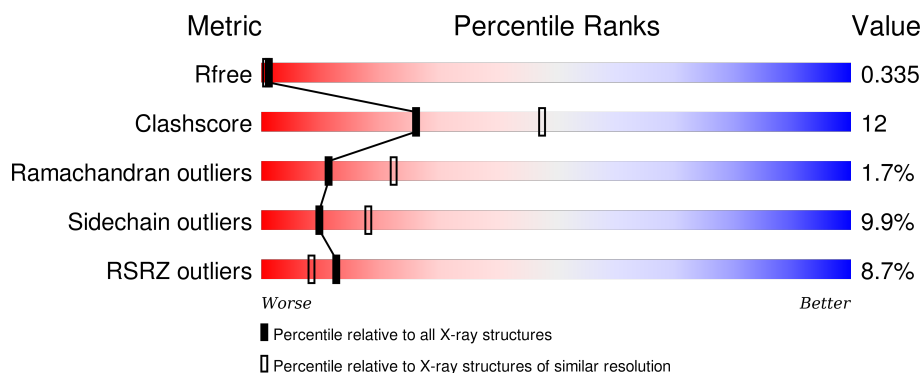
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	<div> <div>8%</div> <div>59%</div> <div>23%</div> <div>5%</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

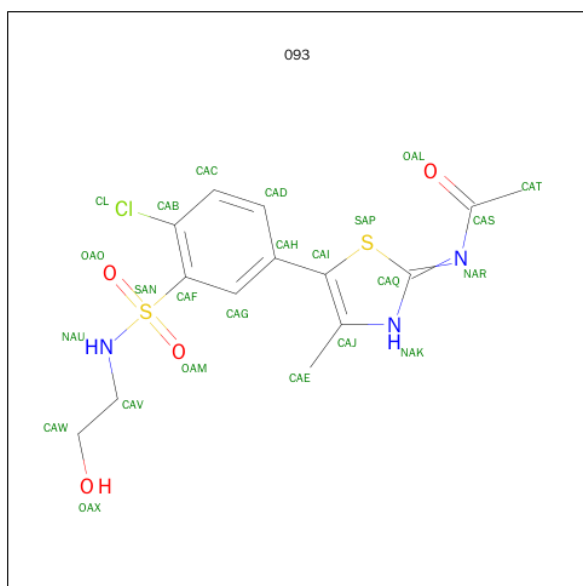
There are 2 unique types of molecules in this entry. The entry contains 6826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	840	6802	4367	1163	1237	35	0	0	1

- Molecule 2 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C<sub>14</sub>H<sub>16</sub>ClN<sub>3</sub>O<sub>4</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	24	14	1	3	4	2	0	0



HIS
SER
ALA
HIS
HIS
HIS
HIS
HIS
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.03Å 68.11Å 106.35Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	71.80 – 2.60 71.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.80-2.60) 99.7 (71.71-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.244 , 0.302 0.280 , 0.335	Depositor DCC
$R_{free}$ test set	1306 reflections (4.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 31752 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 093

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	0.61	9/6947 (0.1%)	0.62	4/9395 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	GLY	C-O	25.64	1.64	1.23
1	A	402	LYS	CG-CD	9.22	1.83	1.52
1	A	402	LYS	CE-NZ	9.07	1.71	1.49
1	A	411	ASN	CG-ND2	8.69	1.54	1.32
1	A	918	GLU	CD-OE2	7.38	1.33	1.25
1	A	489	GLY	CA-C	7.17	1.63	1.51
1	A	366	ARG	CZ-NH1	7.07	1.42	1.33
1	A	364	LYS	CE-NZ	6.88	1.66	1.49
1	A	918	GLU	CD-OE1	5.36	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ARG	NE-CZ-NH2	10.88	125.74	120.30
1	A	489	GLY	CA-C-O	-8.88	104.62	120.60
1	A	575	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	409	LEU	CB-CG-CD2	5.34	120.07	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6802	0	6845	164	0
2	A	24	0	16	4	0
All	All	6826	0	6861	168	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 12.

All (168) 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:402:LYS:CG	1:A:402:LYS:CD	1.83	1.54
1:A:402:LYS:CE	1:A:402:LYS:NZ	1.71	1.54
1:A:489:GLY:C	1:A:489:GLY:O	1.64	1.32
1:A:935:TYR:O	1:A:939:THR:HB	1.62	0.98
1:A:558:ILE:O	1:A:561:THR:HG22	1.74	0.87
1:A:410:TRP:HB3	1:A:412:VAL:HG23	1.60	0.83
1:A:402:LYS:CB	1:A:402:LYS:CD	2.59	0.79
2:A:2093:093:CAE	2:A:2093:093:HAD	2.12	0.79
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.33	0.77
1:A:568:THR:HG22	1:A:570:GLU:H	1.51	0.76
1:A:1078:LYS:HB3	1:A:1081:THR:HB	1.69	0.74
1:A:402:LYS:CE	1:A:402:LYS:CG	2.66	0.73
1:A:848:LEU:HD12	1:A:851:MET:HE3	1.74	0.70
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.71	0.69
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.73	0.69
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.40	0.69
1:A:887:THR:HG22	1:A:890:LYS:H	1.57	0.69
1:A:808:LYS:HG3	1:A:833:LYS:HE2	1.74	0.69
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.25	0.66
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.79	0.65
1:A:387:ILE:HD12	1:A:418:ILE:HD13	1.79	0.65
1:A:743:GLN:NE2	1:A:876:ILE:HG23	2.12	0.64
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.15	0.64
1:A:1056:THR:HG23	1:A:1056:THR:O	1.98	0.63
1:A:997:THR:HG23	1:A:1001:LYS:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ARG:HH11	1:A:552:ARG:HB2	1.63	0.63
1:A:357:CYS:SG	1:A:358:ASP:N	2.72	0.61
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.82	0.61
1:A:1001:LYS:H	1:A:1076:ARG:HH22	1.50	0.60
1:A:896:VAL:HG21	1:A:903:LYS:HB2	1.83	0.60
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.66	0.59
1:A:1044:SER:O	1:A:1045:LYS:HB3	2.02	0.59
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.85	0.59
1:A:317:GLU:O	1:A:726:THR:HG23	2.03	0.58
1:A:750:LYS:HE3	1:A:834:HIS:O	2.03	0.58
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.85	0.58
1:A:1069:LEU:HD23	1:A:1072:ILE:HD12	1.86	0.57
1:A:947:ARG:NH2	1:A:963:ILE:O	2.36	0.57
1:A:416:PHE:HB3	1:A:418:ILE:HD12	1.87	0.57
2:A:2093:093:HAE3	2:A:2093:093:HAD	1.86	0.57
1:A:464:VAL:HB	1:A:484:MET:HG2	1.87	0.56
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.46	0.56
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.88	0.56
1:A:1031:PHE:HE2	1:A:1048:ILE:HA	1.71	0.56
2:A:2093:093:HAE2	2:A:2093:093:HAD	1.87	0.55
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.88	0.55
1:A:802:LYS:HG3	1:A:812:TRP:HB3	1.88	0.55
1:A:552:ARG:HB2	1:A:552:ARG:NH1	2.22	0.55
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.71	0.54
1:A:652:GLU:OE1	1:A:654:ASP:HB3	2.07	0.54
1:A:939:THR:HG23	1:A:945:GLY:CA	2.38	0.54
1:A:806:SER:O	1:A:808:LYS:O	2.26	0.53
1:A:181:VAL:O	1:A:185:MET:HG3	2.08	0.53
1:A:620:SER:O	1:A:647:LYS:NZ	2.41	0.53
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.44	0.53
1:A:561:THR:HG23	1:A:591:LYS:NZ	2.23	0.53
1:A:839:ARG:HA	1:A:842:MET:HE2	1.91	0.52
1:A:378:ASP:HB2	1:A:404:PHE:HB3	1.91	0.52
1:A:745:VAL:HG22	1:A:770:LYS:HE2	1.92	0.52
1:A:887:THR:CG2	1:A:950:ASP:HA	2.40	0.52
1:A:421:LYS:HE3	1:A:528:ALA:HB3	1.92	0.52
1:A:498:ASN:C	1:A:498:ASN:OD1	2.48	0.52
1:A:848:LEU:HD12	1:A:851:MET:CE	2.39	0.51
1:A:395:CYS:SG	1:A:417:SER:OG	2.58	0.51
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.92	0.51
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:THR:HB	1:A:1046:GLU:HB2	1.93	0.51
2:A:2093:093:CAE	2:A:2093:093:CAD	2.88	0.51
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.93	0.51
1:A:702:GLU:OE1	1:A:839:ARG:NH1	2.45	0.50
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.42	0.50
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.93	0.50
1:A:1000:LYS:H	1:A:1076:ARG:NH1	2.10	0.49
1:A:373:LEU:N	1:A:374:PRO:HD2	2.26	0.49
1:A:569:ALA:O	1:A:573:GLU:HG3	2.12	0.49
1:A:402:LYS:NZ	1:A:402:LYS:CD	2.67	0.49
1:A:220:ILE:N	1:A:235:VAL:O	2.43	0.49
1:A:1078:LYS:O	1:A:1080:TRP:N	2.46	0.49
1:A:480:TYR:O	1:A:517:SER:HA	2.13	0.49
1:A:1089:HIS:C	1:A:1091:VAL:H	2.16	0.49
1:A:1078:LYS:HB3	1:A:1081:THR:CB	2.40	0.49
1:A:525:HIS:HB2	1:A:526:PRO:HD3	1.95	0.49
1:A:161:ASP:OD2	1:A:164:ASP:HB2	2.13	0.48
1:A:735:GLN:O	1:A:739:ILE:HG23	2.13	0.48
1:A:1041:GLN:HA	1:A:1041:GLN:HE21	1.78	0.48
1:A:158:ILE:HG12	1:A:717:LEU:HD13	1.95	0.48
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.96	0.48
1:A:145:GLU:HA	1:A:148:GLN:HE21	1.78	0.48
1:A:774:LEU:HA	1:A:778:GLN:OE1	2.13	0.48
1:A:375:ARG:NH1	1:A:376:ASN:HB2	2.28	0.48
1:A:845:LEU:HD23	1:A:869:CYS:HB3	1.95	0.48
1:A:743:GLN:C	1:A:745:VAL:H	2.16	0.47
1:A:660:LEU:O	1:A:664:VAL:HG23	2.13	0.47
1:A:568:THR:HG22	1:A:570:GLU:N	2.25	0.47
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.44	0.47
1:A:922:GLN:HA	1:A:922:GLN:OE1	2.13	0.47
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.13	0.47
1:A:198:MET:SD	1:A:282:VAL:HG11	2.54	0.47
1:A:622:LEU:HD21	1:A:651:LEU:HG	1.97	0.47
1:A:168:VAL:HG13	1:A:169:HIS:N	2.31	0.46
1:A:1059:LYS:HE3	1:A:1059:LYS:HA	1.97	0.46
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.42	0.46
1:A:395:CYS:HG	1:A:417:SER:HG	1.42	0.46
1:A:489:GLY:O	1:A:489:GLY:CA	2.59	0.46
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.98	0.46
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.81	0.45
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:CYS:HA	1:A:235:VAL:O	2.17	0.45
1:A:1002:THR:HG22	1:A:1007:GLN:HG3	1.98	0.45
1:A:382:PHE:HE2	1:A:398:ARG:HH11	1.62	0.45
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.52	0.45
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.51	0.45
1:A:371:PRO:HG2	1:A:511:GLU:O	2.15	0.45
1:A:480:TYR:HB2	1:A:518:ILE:CG1	2.46	0.45
1:A:641:ARG:NE	1:A:670:GLU:OE1	2.40	0.45
1:A:737:GLN:O	1:A:741:MET:HG3	2.17	0.45
1:A:241:PRO:HD2	1:A:285:THR:O	2.17	0.44
1:A:887:THR:HG21	1:A:950:ASP:HA	2.00	0.44
1:A:548:PRO:CG	1:A:551:LEU:HD12	2.46	0.44
1:A:601:GLN:HG3	1:A:602:GLU:N	2.31	0.44
1:A:764:ILE:HG13	1:A:764:ILE:H	1.59	0.44
1:A:364:LYS:O	1:A:518:ILE:HA	2.17	0.44
1:A:369:ASP:OD1	1:A:369:ASP:N	2.50	0.44
1:A:1056:THR:CG2	1:A:1056:THR:O	2.64	0.44
1:A:147:SER:HA	1:A:319:ARG:HH12	1.83	0.43
1:A:997:THR:HG23	1:A:1001:LYS:CG	2.48	0.43
1:A:903:LYS:HG2	1:A:905:GLU:OE2	2.18	0.43
1:A:945:GLY:HA3	1:A:984:PRO:O	2.19	0.43
1:A:653:ASP:CG	1:A:684:ARG:HH21	2.21	0.43
1:A:960:LEU:HD11	1:A:991:PHE:CE2	2.54	0.43
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.84	0.43
1:A:641:ARG:HE	1:A:670:GLU:CD	2.22	0.43
1:A:433:ILE:HB	1:A:462:TYR:HB2	2.00	0.43
1:A:887:THR:HG23	1:A:950:ASP:HA	2.01	0.42
1:A:960:LEU:HD11	1:A:991:PHE:HE2	1.85	0.42
1:A:629:GLN:HG3	1:A:1029:ILE:HG13	1.97	0.42
1:A:798:ILE:H	1:A:798:ILE:HD12	1.84	0.42
1:A:834:HIS:HB2	1:A:876:ILE:CD1	2.45	0.42
1:A:1052:ARG:HG3	1:A:1053:ASP:N	2.34	0.42
1:A:892:GLN:NE2	1:A:903:LYS:O	2.53	0.42
1:A:497:PHE:HB3	1:A:1041:GLN:NE2	2.34	0.42
1:A:184:ARG:HH21	1:A:321:GLU:CD	2.23	0.42
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.19	0.42
1:A:915:SER:HA	1:A:916:PRO:HD3	1.77	0.42
1:A:205:LYS:O	1:A:206:PRO:O	2.38	0.42
1:A:840:GLN:O	1:A:844:ILE:HG12	2.20	0.42
1:A:253:ALA:O	1:A:254:LYS:HB2	2.20	0.42
1:A:589:TYR:CD2	1:A:593:PHE:HE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:O	1:A:165:VAL:HG12	2.20	0.41
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.50	0.41
1:A:378:ASP:CB	1:A:404:PHE:HB3	2.49	0.41
1:A:389:HIS:O	1:A:392:GLN:HB3	2.20	0.41
1:A:561:THR:HG23	1:A:591:LYS:HZ1	1.85	0.41
1:A:807:LYS:HE3	1:A:808:LYS:HG2	2.03	0.41
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.55	0.41
1:A:387:ILE:HD12	1:A:418:ILE:CD1	2.49	0.41
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.56	0.41
1:A:1021:ARG:NE	1:A:1056:THR:HG22	2.34	0.41
1:A:475:LEU:HD21	1:A:522:ASN:HB2	2.02	0.41
1:A:233:ILE:HG22	1:A:235:VAL:HG23	2.02	0.41
1:A:651:LEU:HD22	1:A:655:ASP:HB3	2.01	0.41
1:A:271:VAL:CG2	1:A:282:VAL:HG12	2.51	0.41
1:A:583:LEU:HD22	1:A:610:LEU:HD22	2.02	0.41
1:A:839:ARG:HG2	1:A:842:MET:HE2	2.04	0.40
1:A:774:LEU:HD22	1:A:779:LEU:HD13	2.01	0.40
1:A:1036:MET:HA	1:A:1042:LEU:HD11	2.03	0.40
1:A:580:TYR:HE2	1:A:613:ARG:HD3	1.86	0.40
1:A:904:ASP:N	1:A:904:ASP:OD2	2.55	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	822/966 (85%)	745 (91%)	63 (8%)	14 (2%)	11 22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO

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Mol	Chain	Res	Type
1	A	379	LEU
1	A	897	GLY
1	A	1040	PRO
1	A	1045	LYS
1	A	1079	GLY
1	A	206	PRO
1	A	758	ASP
1	A	319	ARG
1	A	949	ASN
1	A	1000	LYS
1	A	1090	LEU
1	A	227	SER
1	A	526	PRO

### 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	754/864 (87%)	679 (90%)	75 (10%)	10	18

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	163	THR
1	A	168	VAL
1	A	214	LYS
1	A	219	CYS
1	A	220	ILE
1	A	226	ARG
1	A	250	THR
1	A	281	LEU
1	A	287	ILE
1	A	358	ASP
1	A	359	ARG
1	A	373	LEU

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Mol	Chain	Res	Type
1	A	375	ARG
1	A	378	ASP
1	A	381	VAL
1	A	406	GLU
1	A	418	ILE
1	A	464	VAL
1	A	477	ARG
1	A	521	ASP
1	A	544	ARG
1	A	552	ARG
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	647	LYS
1	A	652	GLU
1	A	682	LEU
1	A	705	GLN
1	A	717	LEU
1	A	739	ILE
1	A	748	ASP
1	A	755	GLU
1	A	756	LYS
1	A	764	ILE
1	A	766	GLN
1	A	767	LEU
1	A	769	GLN
1	A	774	LEU
1	A	799	GLU
1	A	804	MET
1	A	807	LYS
1	A	811	LEU
1	A	825	ASN
1	A	832	PHE
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	863	CYS
1	A	865	LEU
1	A	899	THR

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Mol	Chain	Res	Type
1	A	905	GLU
1	A	913	GLU
1	A	927	ARG
1	A	939	THR
1	A	957	THR
1	A	967	HIS
1	A	982	ARG
1	A	1002	THR
1	A	1026	LEU
1	A	1041	GLN
1	A	1042	LEU
1	A	1043	THR
1	A	1045	LYS
1	A	1052	ARG
1	A	1056	THR
1	A	1059	LYS
1	A	1062	GLU
1	A	1078	LYS
1	A	1088	LEU
1	A	1091	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	169	HIS
1	A	225	HIS
1	A	304	HIS
1	A	392	GLN
1	A	512	ASN
1	A	550	GLN
1	A	565	ASN
1	A	601	GLN
1	A	646	GLN
1	A	705	GLN
1	A	734	GLN
1	A	743	GLN
1	A	951	ASN
1	A	959	ASN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	093	A	2093	-	21,25,25	2.92	4 (19%)	24,36,36	2.33	5 (20%)

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	093	A	2093	-	-	0/17/19/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2093	093	CAH-CAI	-7.78	1.40	1.48
2	A	2093	093	SAN-NAU	-6.61	1.52	1.61
2	A	2093	093	OAO-SAN	5.77	1.49	1.43
2	A	2093	093	OAM-SAN	5.80	1.49	1.43



All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2093	093	OAO-SAN-OAM	-8.78	107.89	119.54
2	A	2093	093	CAB-CAF-SAN	-2.68	121.66	123.30
2	A	2093	093	CAW-CAV-NAU	-2.30	106.05	110.34
2	A	2093	093	CAF-SAN-NAU	3.56	112.68	107.92
2	A	2093	093	CAQ-NAR-CAS	3.98	126.76	115.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2093	093	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	840/966 (86%)	0.75	73 (8%) 13 8	31, 61, 84, 104	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1092	LEU	6.1
1	A	1044	SER	4.8
1	A	404	PHE	4.6
1	A	895	THR	4.6
1	A	528	ALA	4.1
1	A	375	ARG	4.1
1	A	461	LEU	4.0
1	A	902	PHE	3.8
1	A	403	PRO	3.8
1	A	811	LEU	3.6
1	A	322	GLU	3.6
1	A	381	VAL	3.6
1	A	376	ASN	3.5
1	A	305	VAL	3.5
1	A	374	PRO	3.5
1	A	1045	LYS	3.4
1	A	991	PHE	3.3
1	A	898	ASN	3.3
1	A	210	TYR	3.2
1	A	757	TYR	3.2
1	A	986	VAL	3.2
1	A	460	LEU	3.2
1	A	1086	TRP	3.1
1	A	1089	HIS	3.1
1	A	987	LEU	3.1
1	A	281	LEU	3.0
1	A	545	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	813	LEU	2.9
1	A	907	LEU	2.9
1	A	766	GLN	2.8
1	A	211	LEU	2.8
1	A	990	ASP	2.8
1	A	377	THR	2.8
1	A	767	LEU	2.8
1	A	771	LEU	2.7
1	A	362	ARG	2.7
1	A	303	ILE	2.6
1	A	998	SER	2.6
1	A	997	THR	2.6
1	A	1006	PHE	2.6
1	A	223	VAL	2.5
1	A	359	ARG	2.5
1	A	1069	LEU	2.4
1	A	178	ARG	2.4
1	A	253	ALA	2.4
1	A	896	VAL	2.4
1	A	613	ARG	2.3
1	A	401	PRO	2.3
1	A	489	GLY	2.3
1	A	1007	GLN	2.3
1	A	1055	LEU	2.2
1	A	1009	PHE	2.2
1	A	783	PHE	2.2
1	A	559	ILE	2.1
1	A	996	GLY	2.1
1	A	772	GLU	2.1
1	A	378	ASP	2.1
1	A	760	SER	2.1
1	A	879	ILE	2.1
1	A	916	PRO	2.1
1	A	198	MET	2.1
1	A	1087	PHE	2.1
1	A	475	LEU	2.1
1	A	175	PHE	2.1
1	A	823	LEU	2.1
1	A	293	VAL	2.1
1	A	994	VAL	2.1
1	A	462	TYR	2.1
1	A	903	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	522	ASN	2.1
1	A	1040	PRO	2.1
1	A	1083	GLN	2.0
1	A	520	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	093	A	2093	24/24	0.85	0.26	0.89	77,79,79,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.