Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	4XX5
Title	:	Structure of PI3K gamma in complex with an inhibitor
Authors	:	Collier, P.N.; Messersmith, D.; Le Tiran, A.; Bandarage, U.K.; Boucher, C.; Come, J.; Cottrell, K.M.; Damagnez, V.; Doran, J.D.; Griffith, J.P.; Khare-Pandit, S.; Krueger, E.B.; Ledeboer, M.W.; Ledford, B.; Liao, Y.; Mahajan, S.; Moody, C.S.; Wang, T.; Xu, J.; Aronov, A.M.
Deposited on	:	2015-01-29
Resolution	:	2.76 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		9
Ramachandran outliers		2.4%
Sidechain outliers		11.0%
RSRZ outliers		5.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
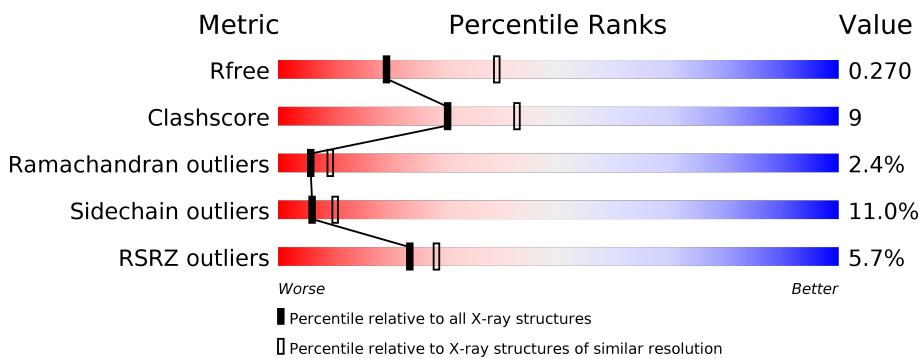
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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 <=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	5% [bar: 61% / 23% / · / 13%]

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6870 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	843	6844	4395	1170	1244	35	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P48736
A	459	ARG	GLN	conflict	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is N-[5-(5-methoxypyridin-3-yl)-4,5,6,7-tetrahydro[1,3]thiazolo[5,4-c]pyridin-2-yl] acetamide (three-letter code: 43R) (formula: $C_{14}H_{16}N_4O_2S$).
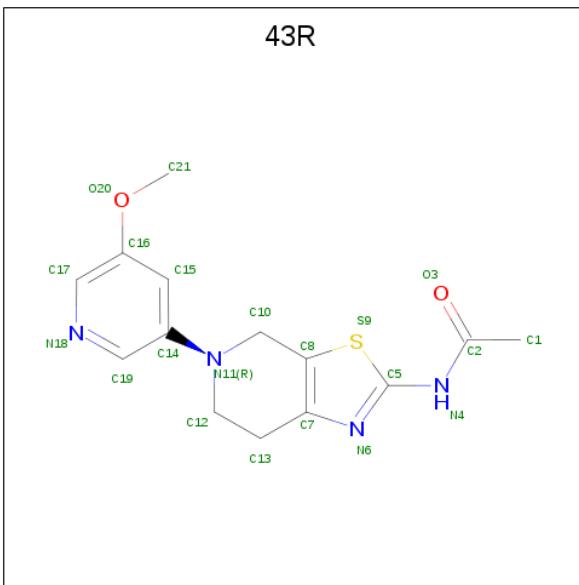
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	14	4	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		

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 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform
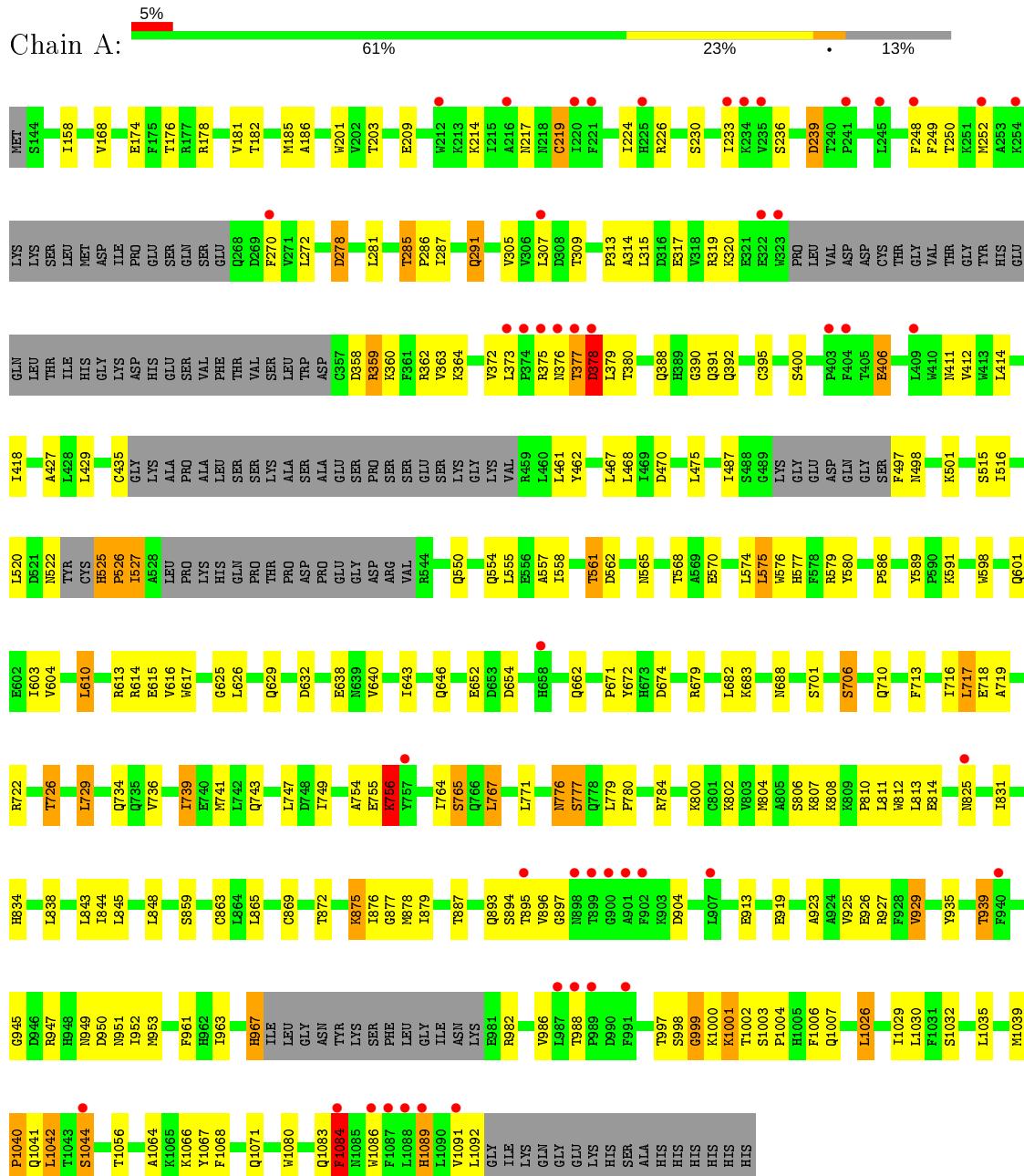
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.44Å 67.42Å 106.70Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	106.18 – 2.76 44.87 – 2.76	Depositor EDS
% Data completeness (in resolution range)	72.5 (106.18-2.76) 72.5 (44.87-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.33 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.198 , 0.274 0.202 , 0.270	Depositor DCC
R_{free} test set	959 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	75.6	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 83.2	EDS
L-test for twinning [2]	$<|L|>=0.50, <L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6870	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: 43R

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	0.55	1/6992 (0.0%)	0.74	1/9457 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1086	TRP	CB-CG	5.44	1.60	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	904	ASP	CB-CG-OD1	6.16	123.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	TRP	Peptide

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	6844	0	6886	128	0
2	A	21	0	16	1	0
3	A	5	0	0	2	0
All	All	6870	0	6902	128	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 9.

All (128) 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:893:GLN:HA	1:A:897:GLY:CA	1.95	0.96
1:A:640:VAL:O	1:A:643:ILE:HG12	1.74	0.88
1:A:893:GLN:HA	1:A:897:GLY:HA2	1.64	0.76
1:A:475:LEU:HD21	1:A:522:ASN:HB2	1.68	0.75
1:A:497:PHE:N	1:A:1044:SER:HG	1.85	0.74
1:A:1080:TRP:O	1:A:1084:PHE:HB2	1.89	0.73
1:A:625:GLY:O	1:A:629:GLN:HG3	1.92	0.69
1:A:1042:LEU:O	1:A:1042:LEU:HD22	1.94	0.66
1:A:554:GLN:O	1:A:558:ILE:HD12	1.96	0.65
1:A:248:PHE:C	1:A:250:THR:H	1.98	0.65
1:A:378:ASP:OD1	1:A:378:ASP:N	2.32	0.62
1:A:555:LEU:HD11	1:A:575:LEU:HD12	1.82	0.61
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.83	0.60
1:A:248:PHE:C	1:A:250:THR:N	2.54	0.60
1:A:811:LEU:O	1:A:831:ILE:HA	2.03	0.58
1:A:359:ARG:HG3	1:A:360:LYS:O	2.03	0.58
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.85	0.58
1:A:997:THR:HG23	1:A:1001:LYS:HG3	1.87	0.57
1:A:182:THR:O	1:A:186:ALA:N	2.34	0.56
1:A:947:ARG:NH2	1:A:963:ILE:O	2.37	0.56
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.87	0.56
1:A:951:ASN:ND2	3:A:1302:HOH:O	2.39	0.56
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.36	0.56
1:A:576:TRP:CZ2	1:A:603:ILE:HG23	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:GLN:O	1:A:747:LEU:HD12	2.06	0.55
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.89	0.55
1:A:467:LEU:HD13	1:A:672:TYR:CE1	2.42	0.55
1:A:935:TYR:O	1:A:939:THR:HB	2.07	0.55
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.90	0.54
1:A:1042:LEU:N	1:A:1042:LEU:HD13	2.22	0.54
1:A:1064:ALA:O	1:A:1067:TYR:HB3	2.08	0.54
1:A:893:GLN:HA	1:A:897:GLY:N	2.23	0.53
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.91	0.53
1:A:736:VAL:O	1:A:739:ILE:HD13	2.08	0.53
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.90	0.52
1:A:879:ILE:HG21	2:A:1201:43R:H1	1.91	0.52
1:A:706:SER:O	1:A:710:GLN:HB3	2.09	0.52
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.91	0.52
1:A:598:TRP:CE3	1:A:604:VAL:HG22	2.45	0.52
1:A:364:LYS:HA	1:A:412:VAL:O	2.10	0.51
1:A:362:ARG:HA	1:A:414:LEU:O	2.09	0.51
1:A:726:THR:N	1:A:729:LEU:HD12	2.25	0.51
1:A:248:PHE:O	1:A:250:THR:N	2.44	0.51
1:A:1035:LEU:HA	1:A:1039:MET:CG	2.41	0.51
1:A:734:GLN:NE2	1:A:780:PRO:HB3	2.26	0.51
1:A:390:GLY:C	1:A:392:GLN:H	2.14	0.51
1:A:800:LYS:HB3	1:A:814:GLU:OE1	2.11	0.51
1:A:998:SER:O	1:A:999:GLY:C	2.49	0.51
1:A:887:THR:CG2	1:A:950:ASP:HA	2.42	0.50
1:A:526:PRO:O	1:A:527:ILE:HG22	2.12	0.50
1:A:894:SER:OG	1:A:895:THR:N	2.44	0.49
1:A:363:VAL:HG13	1:A:363:VAL:O	2.12	0.49
1:A:498:ASN:O	1:A:501:LYS:HB2	2.12	0.49
1:A:734:GLN:HE22	1:A:780:PRO:HB3	1.78	0.49
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.86	0.48
1:A:174:GLU:O	1:A:178:ARG:HG2	2.12	0.48
1:A:802:LYS:HG3	1:A:812:TRP:HB3	1.95	0.48
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.14	0.48
1:A:925:VAL:O	1:A:929:VAL:HG23	2.15	0.47
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.96	0.47
1:A:181:VAL:O	1:A:185:MET:HG3	2.14	0.47
1:A:674:ASP:OD1	1:A:679:ARG:NE	2.47	0.47
1:A:755:GLU:O	1:A:756:LYS:C	2.54	0.47
1:A:806:SER:HB2	1:A:810:PRO:HD3	1.96	0.47
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:ILE:O	1:A:765:SER:C	2.53	0.46
1:A:467:LEU:HD11	1:A:671:PRO:O	2.16	0.46
1:A:952:ILE:HD11	1:A:986:VAL:HG21	1.98	0.46
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.50	0.46
1:A:562:ASP:OD1	1:A:565:ASN:N	2.48	0.46
1:A:568:THR:HG22	1:A:570:GLU:H	1.80	0.45
1:A:580:TYR:CE1	1:A:610:LEU:HD23	2.51	0.45
1:A:380:THR:O	1:A:435:CYS:HB3	2.16	0.45
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.98	0.45
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.16	0.45
1:A:278:ASP:HB2	1:A:784:ARG:HH12	1.82	0.45
1:A:1056:THR:HG23	1:A:1056:THR:O	2.17	0.45
1:A:576:TRP:O	1:A:577:HIS:C	2.54	0.45
1:A:967:HIS:CD2	3:A:1303:HOH:O	2.69	0.45
1:A:475:LEU:HD21	1:A:522:ASN:CB	2.43	0.45
1:A:767:LEU:O	1:A:771:LEU:HG	2.17	0.45
1:A:579:ARG:HB2	1:A:610:LEU:HD11	1.99	0.45
1:A:767:LEU:HD12	1:A:802:LYS:HA	1.98	0.44
1:A:285:THR:HG22	1:A:286:PRO:HD2	2.00	0.44
1:A:554:GLN:O	1:A:557:ALA:HB3	2.17	0.44
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.47	0.44
1:A:953:MET:O	1:A:961:PHE:N	2.45	0.44
1:A:233:ILE:HD12	1:A:233:ILE:N	2.32	0.44
1:A:313:PRO:C	1:A:315:LEU:H	2.20	0.44
1:A:380:THR:O	1:A:435:CYS:CB	2.66	0.44
1:A:632:ASP:OD1	1:A:632:ASP:C	2.57	0.43
1:A:614:ARG:NH1	1:A:643:ILE:HG22	2.34	0.43
1:A:652:GLU:HG3	1:A:654:ASP:HB3	2.00	0.43
1:A:614:ARG:O	1:A:615:GLU:C	2.57	0.43
1:A:561:THR:HG22	1:A:565:ASN:HB3	1.99	0.43
1:A:713:PHE:HA	1:A:716:ILE:HD12	2.01	0.43
1:A:377:THR:O	1:A:378:ASP:C	2.57	0.43
1:A:806:SER:O	1:A:808:LYS:O	2.36	0.43
1:A:470:ASP:C	1:A:470:ASP:OD1	2.57	0.42
1:A:718:GLU:O	1:A:722:ARG:HG3	2.19	0.42
1:A:224:ILE:O	1:A:230:SER:HA	2.19	0.42
1:A:236:SER:O	1:A:239:ASP:HB2	2.19	0.42
1:A:923:ALA:O	1:A:926:GLU:HB3	2.19	0.42
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.85	0.42
1:A:313:PRO:C	1:A:315:LEU:N	2.72	0.42
1:A:1006:PHE:O	1:A:1007:GLN:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASN:O	1:A:411:ASN:CG	2.59	0.41
1:A:844:ILE:O	1:A:848:LEU:HD13	2.20	0.41
1:A:217:ASN:ND2	1:A:219:CYS:SG	2.93	0.41
1:A:270:PHE:CD2	1:A:307:LEU:HD21	2.55	0.41
1:A:388:GLN:O	1:A:427:ALA:HA	2.20	0.41
1:A:158:ILE:HG12	1:A:717:LEU:HD13	2.02	0.41
1:A:726:THR:HA	1:A:729:LEU:HB2	2.01	0.41
1:A:461:LEU:HB3	1:A:462:TYR:CD1	2.55	0.41
1:A:575:LEU:HD21	1:A:591:LYS:HB3	2.01	0.41
1:A:939:THR:HG23	1:A:945:GLY:HA2	2.02	0.41
1:A:1089:HIS:C	1:A:1091:VAL:N	2.72	0.41
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	2.02	0.41
1:A:224:ILE:CD1	1:A:233:ILE:HD13	2.50	0.41
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.56	0.41
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.68	0.41
1:A:741:MET:SD	1:A:779:LEU:HD12	2.61	0.41
1:A:812:TRP:C	1:A:813:LEU:HD23	2.40	0.41
1:A:878:MET:C	1:A:879:ILE:HG13	2.42	0.41
1:A:1003:SER:HB2	1:A:1004:PRO:CD	2.51	0.40
1:A:516:ILE:HG23	1:A:516:ILE:O	2.21	0.40
1:A:395:CYS:HB3	1:A:418:ILE:HD11	2.02	0.40
1:A:716:ILE:O	1:A:719:ALA:HB3	2.22	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	827/966 (86%)	734 (89%)	73 (9%)	20 (2%)	6 9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	ILE
1	A	561	THR
1	A	726	THR
1	A	754	ALA
1	A	1000	LYS
1	A	1040	PRO
1	A	249	PHE
1	A	317	GLU
1	A	378	ASP
1	A	391	GLN
1	A	406	GLU
1	A	756	LYS
1	A	776	ASN
1	A	999	GLY
1	A	314	ALA
1	A	526	PRO
1	A	638	GLU
1	A	1084	PHE
1	A	875	LYS
1	A	777	SER

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	757/864 (88%)	674 (89%)	83 (11%)	6 10

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	VAL
1	A	203	THR
1	A	214	LYS
1	A	219	CYS
1	A	226	ARG
1	A	239	ASP
1	A	252	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	278	ASP
1	A	281	LEU
1	A	285	THR
1	A	287	ILE
1	A	291	GLN
1	A	309	THR
1	A	319	ARG
1	A	320	LYS
1	A	358	ASP
1	A	359	ARG
1	A	372	VAL
1	A	373	LEU
1	A	375	ARG
1	A	376	ASN
1	A	377	THR
1	A	378	ASP
1	A	379	LEU
1	A	400	SER
1	A	406	GLU
1	A	487	ILE
1	A	515	SER
1	A	520	LEU
1	A	525	HIS
1	A	550	GLN
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	616	VAL
1	A	626	LEU
1	A	646	GLN
1	A	662	GLN
1	A	682	LEU
1	A	683	LYS
1	A	688	ASN
1	A	701	SER
1	A	706	SER
1	A	717	LEU
1	A	729	LEU
1	A	739	ILE
1	A	749	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	756	LYS
1	A	765	SER
1	A	767	LEU
1	A	776	ASN
1	A	777	SER
1	A	804	MET
1	A	807	LYS
1	A	825	ASN
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	865	LEU
1	A	869	CYS
1	A	875	LYS
1	A	896	VAL
1	A	913	GLU
1	A	919	GLU
1	A	929	VAL
1	A	939	THR
1	A	967	HIS
1	A	982	ARG
1	A	988	THR
1	A	1001	LYS
1	A	1002	THR
1	A	1026	LEU
1	A	1029	ILE
1	A	1032	SER
1	A	1041	GLN
1	A	1042	LEU
1	A	1044	SER
1	A	1066	LYS
1	A	1084	PHE
1	A	1089	HIS
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	217	ASN
1	A	218	ASN
1	A	231	GLN

Continued from previous page...

Mol	Chain	Res	Type
1	A	291	GLN
1	A	304	HIS
1	A	432	GLN
1	A	565	ASN
1	A	601	GLN
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	840	GLN
1	A	967	HIS
1	A	1007	GLN
1	A	1041	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	43R	A	1201	-	20,23,23	1.25	3 (15%)	20,32,32	2.05	8 (40%)

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	43R	A	1201	-	-	0/8/19/19	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	43R	C8-C7	-3.23	1.36	1.42
2	A	1201	43R	C5-N4	2.31	1.40	1.36
2	A	1201	43R	C17-C16	2.07	1.41	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	43R	C10-N11-C14	-5.29	109.50	117.87
2	A	1201	43R	C1-C2-N4	3.53	120.16	114.98
2	A	1201	43R	O3-C2-C1	-2.74	116.96	122.06
2	A	1201	43R	C19-N18-C17	2.62	121.06	117.48
2	A	1201	43R	C12-N11-C14	-2.49	111.37	118.09
2	A	1201	43R	C12-C13-C7	-2.12	109.09	113.00
2	A	1201	43R	C8-C10-N11	-2.11	110.51	112.72
2	A	1201	43R	C13-C12-N11	2.05	117.26	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	43R	1	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 then 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.

Ligand 43R A 1201
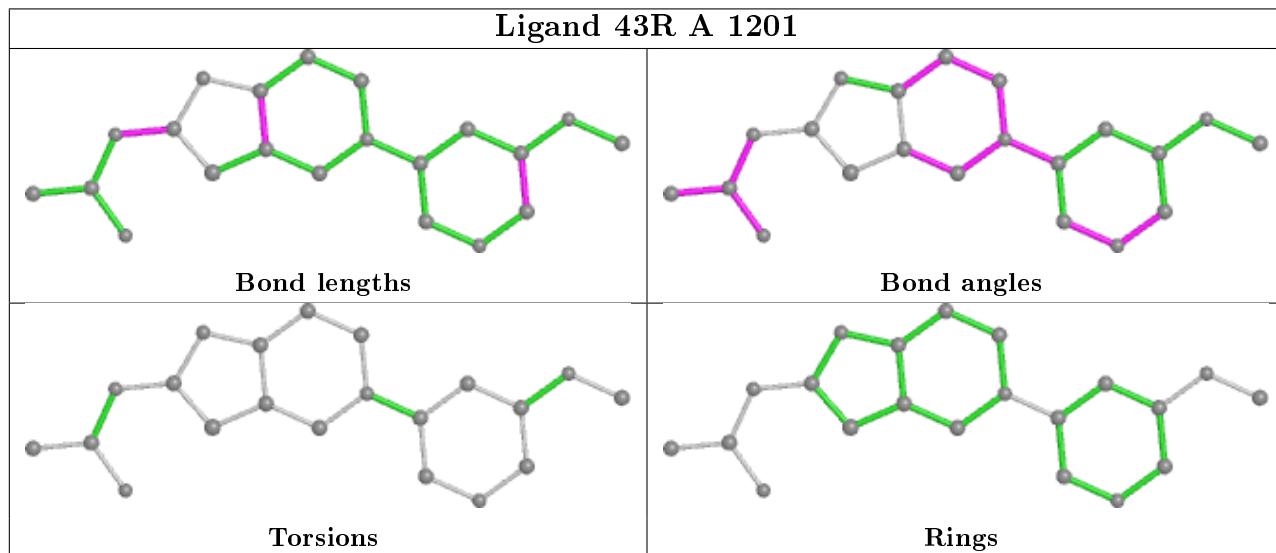
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	843/966 (87%)	0.10	48 (5%)	23	28	28, 55, 98, 141	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	8.6
1	A	899	THR	7.6
1	A	1088	LEU	6.3
1	A	322	GLU	6.0
1	A	404	PHE	5.7
1	A	900	GLY	5.1
1	A	248	PHE	5.0
1	A	323	TRP	5.0
1	A	901	ALA	4.7
1	A	221	PHE	4.7
1	A	403	PRO	4.6
1	A	374	PRO	4.5
1	A	991	PHE	4.2
1	A	1086	TRP	4.2
1	A	307	LEU	4.0
1	A	902	PHE	4.0
1	A	757	TYR	3.5
1	A	1087	PHE	3.3
1	A	233	ILE	3.3
1	A	252	MET	3.2
1	A	241	PRO	3.2
1	A	1091	VAL	3.2
1	A	898	ASN	3.2
1	A	234	LYS	3.2
1	A	376	ASN	3.1
1	A	825	ASN	3.1
1	A	220	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	3.0
1	A	1089	HIS	3.0
1	A	375	ARG	2.9
1	A	212	TRP	2.8
1	A	409	LEU	2.8
1	A	377	THR	2.8
1	A	987	LEU	2.7
1	A	235	VAL	2.6
1	A	270	PHE	2.5
1	A	1084	PHE	2.5
1	A	373	LEU	2.5
1	A	225	HIS	2.4
1	A	378	ASP	2.4
1	A	895	THR	2.3
1	A	940	PHE	2.2
1	A	254	LYS	2.1
1	A	245	LEU	2.1
1	A	988	THR	2.1
1	A	907	LEU	2.1
1	A	658	HIS	2.0
1	A	989	PRO	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, 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(Å^2)	Q<0.9
2	43R	A	1201	21/21	0.97	0.17	58,69,88,90	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 43R A 1201:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.