



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:27 am GMT

PDB ID : 4XZ4  
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 : 2015-02-03  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

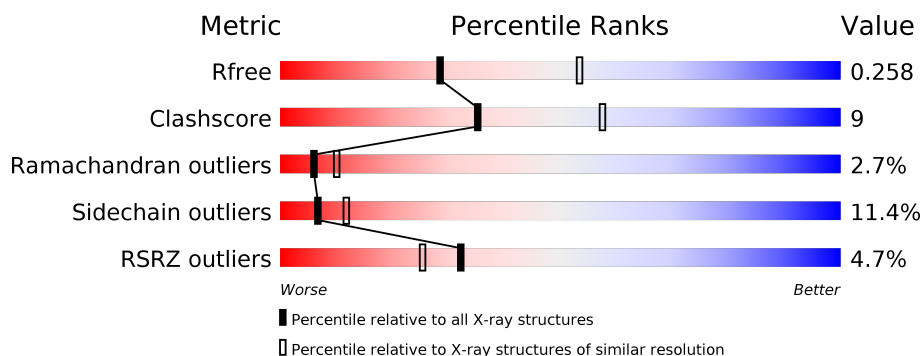
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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>4%</div> <div>60%</div> <div>23%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6871 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.

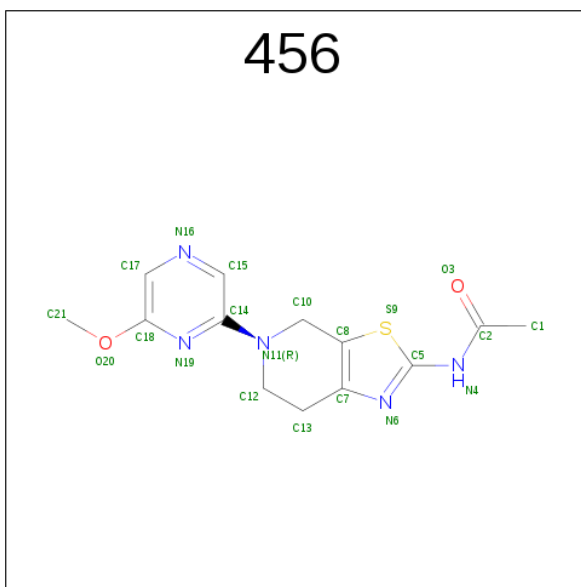
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	843	Total	C	N	O	S	0	0	0
			6844	4395	1170	1244	35			

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-(6-methoxypyrazin-2-yl)-4,5,6,7-tetrahydro[1,3]thiazolo[5,4-c]pyridin-2-yl]acetamide (three-letter code: 456) (formula: C<sub>13</sub>H<sub>15</sub>N<sub>5</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	13	5	2	1		

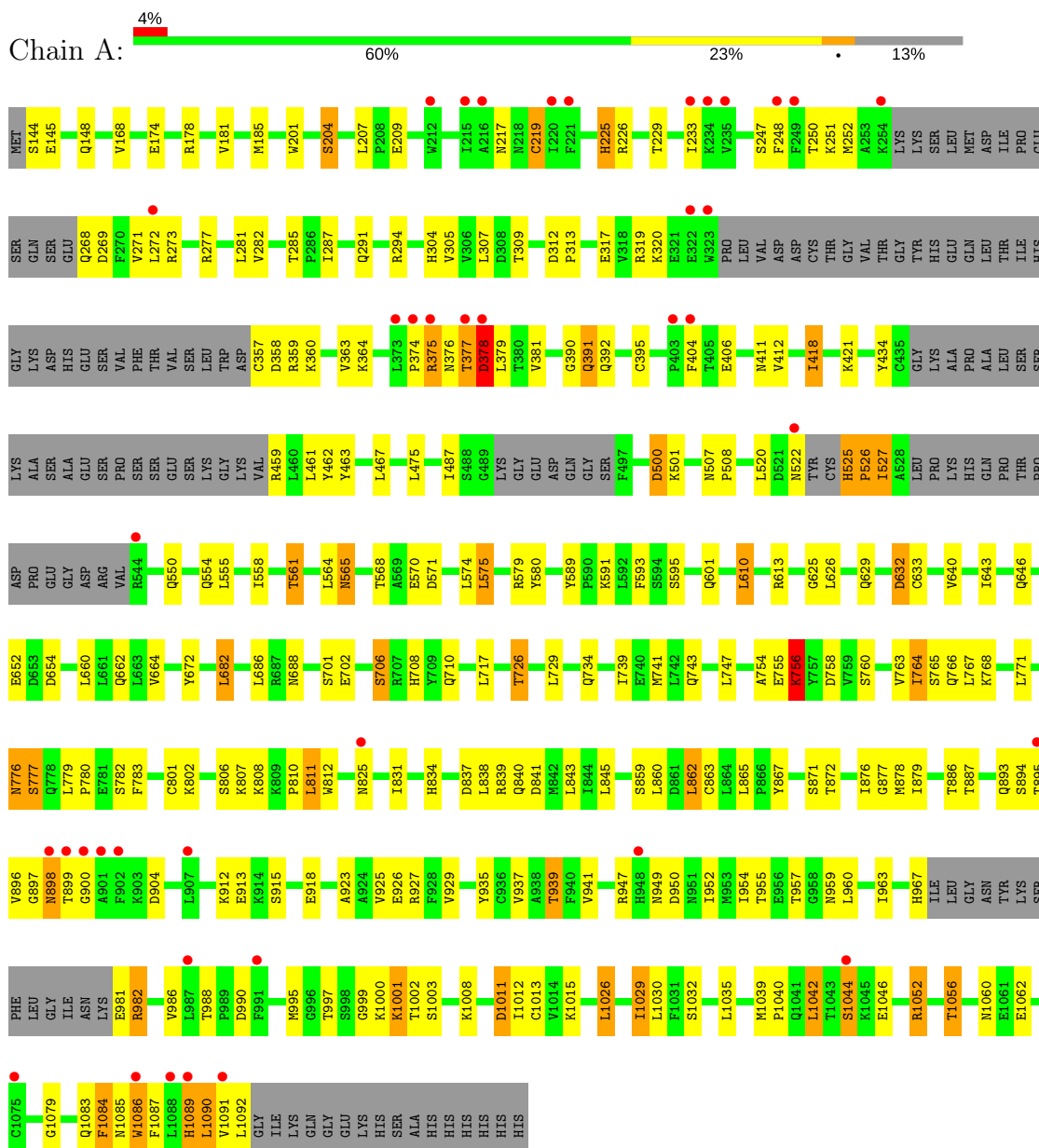
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

### 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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.70Å 67.18Å 106.34Å 90.00° 95.89° 90.00°	Depositor
Resolution (Å)	44.77 – 2.60 40.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	73.1 (44.77-2.60) 73.1 (40.80-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.199 , 0.262 0.200 , 0.258	Depositor DCC
$R_{free}$ test set	1170 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.6	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 72.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 456

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	0.63	2/6992 (0.0%)	0.80	3/9457 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1086	TRP	CB-CG	6.03	1.61	1.50
1	A	904	ASP	CB-CG	5.12	1.62	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	904	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	632	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	A	500	ASP	CB-CG-OD2	-5.07	113.74	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 ⓘ

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	15	1	0
3	A	6	0	0	0	0
All	All	6871	0	6901	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	1.88	1.03
1:A:893:GLN:HA	1:A:897:GLY:HA2	1.61	0.81
1:A:181:VAL:O	1:A:185:MET:HG3	1.87	0.74
1:A:947:ARG:NH2	1:A:963:ILE:O	2.20	0.74
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.70	0.71
1:A:475:LEU:HD21	1:A:522:ASN:HB2	1.74	0.70
1:A:995:MET:O	1:A:1003:SER:OG	2.10	0.70
1:A:893:GLN:HA	1:A:897:GLY:HA3	1.75	0.69
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.76	0.67
1:A:625:GLY:O	1:A:629:GLN:HG3	1.94	0.67
1:A:925:VAL:O	1:A:929:VAL:HG23	1.95	0.66
1:A:1042:LEU:O	1:A:1042:LEU:HD22	1.96	0.66
1:A:640:VAL:O	1:A:643:ILE:HG12	1.96	0.65
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.27	0.65
1:A:1011:ASP:OD1	1:A:1015:LYS:NZ	2.21	0.63
1:A:554:GLN:O	1:A:558:ILE:HD12	2.00	0.61
1:A:421:LYS:HE3	1:A:527:ILE:HD12	1.83	0.60
1:A:555:LEU:HD11	1:A:575:LEU:HD12	1.82	0.60
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.31	0.60
1:A:923:ALA:O	1:A:926:GLU:HB3	2.02	0.60
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.85	0.59
1:A:561:THR:HG22	1:A:565:ASN:HB3	1.85	0.58
1:A:378:ASP:OD1	1:A:378:ASP:N	2.38	0.57
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.88	0.55
1:A:359:ARG:HG3	1:A:360:LYS:O	2.08	0.54
1:A:1086:TRP:HE3	1:A:1087:PHE:HA	1.73	0.54
1:A:1089:HIS:C	1:A:1091:VAL:N	2.61	0.54
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.90	0.54
1:A:233:ILE:HD12	1:A:233:ILE:N	2.23	0.53
1:A:632:ASP:C	1:A:632:ASP:OD1	2.47	0.53
1:A:726:THR:HA	1:A:729:LEU:HB2	1.91	0.53
1:A:894:SER:OG	1:A:895:THR:N	2.43	0.52
1:A:1060:ASN:OD1	1:A:1062:GLU:HB2	2.09	0.52
1:A:811:LEU:O	1:A:831:ILE:HA	2.09	0.52
1:A:893:GLN:HA	1:A:897:GLY:N	2.25	0.52
1:A:952:ILE:HD11	1:A:986:VAL:HG21	1.92	0.52
1:A:248:PHE:C	1:A:250:THR:N	2.62	0.52
1:A:652:GLU:HG3	1:A:654:ASP:HB3	1.92	0.52
1:A:204:SER:OG	1:A:652:GLU:OE2	2.14	0.51
1:A:461:LEU:HB3	1:A:462:TYR:CD1	2.46	0.51
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.92	0.51
1:A:364:LYS:HA	1:A:412:VAL:O	2.10	0.51
1:A:734:GLN:NE2	1:A:780:PRO:HB3	2.26	0.51
1:A:579:ARG:HB2	1:A:610:LEU:HD11	1.92	0.50
1:A:760:SER:OG	1:A:763:VAL:HG23	2.11	0.50
1:A:768:LYS:HE2	1:A:801:CYS:O	2.11	0.50
1:A:981:GLU:N	1:A:982:ARG:NH2	2.59	0.50
1:A:568:THR:HG22	1:A:570:GLU:H	1.77	0.50
1:A:580:TYR:CE1	1:A:610:LEU:HD23	2.48	0.49
1:A:467:LEU:HD13	1:A:672:TYR:CE1	2.47	0.49
1:A:726:THR:N	1:A:729:LEU:HD12	2.26	0.49
1:A:706:SER:O	1:A:710:GLN:HB3	2.12	0.49
1:A:390:GLY:C	1:A:392:GLN:H	2.15	0.49
1:A:802:LYS:HG3	1:A:812:TRP:HB3	1.93	0.49
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.61	0.49
1:A:250:THR:O	1:A:250:THR:HG22	2.12	0.49
1:A:434:TYR:HA	1:A:459:ARG:O	2.12	0.48
1:A:955:THR:OG1	1:A:957:THR:HG22	2.13	0.48
1:A:174:GLU:O	1:A:178:ARG:HG2	2.13	0.48
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.46	0.48
1:A:1056:THR:HG23	1:A:1056:THR:O	2.14	0.48
1:A:1086:TRP:CE3	1:A:1087:PHE:HA	2.49	0.47
1:A:589:TYR:O	1:A:593:PHE:CD2	2.68	0.47
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.14	0.47
1:A:935:TYR:O	1:A:939:THR:HB	2.15	0.47
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.97	0.47
1:A:802:LYS:CG	1:A:812:TRP:HB3	2.45	0.47
1:A:743:GLN:O	1:A:747:LEU:HD12	2.15	0.47
1:A:1085:ASN:O	1:A:1086:TRP:C	2.54	0.46
1:A:363:VAL:HG13	1:A:363:VAL:O	2.15	0.46
1:A:887:THR:CG2	1:A:950:ASP:HA	2.46	0.46
1:A:1086:TRP:CE3	1:A:1087:PHE:CD2	3.04	0.45
1:A:879:ILE:HG21	2:A:1201:456:H6	1.98	0.45
1:A:741:MET:SD	1:A:779:LEU:HD12	2.57	0.45
1:A:755:GLU:O	1:A:756:LYS:C	2.55	0.45
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.46	0.45
1:A:568:THR:HG22	1:A:570:GLU:N	2.31	0.45
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	1.99	0.45
1:A:1089:HIS:O	1:A:1091:VAL:N	2.49	0.45
1:A:273:ARG:O	1:A:305:VAL:HG13	2.17	0.45
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.99	0.44
1:A:375:ARG:NH1	1:A:377:THR:OG1	2.44	0.44
1:A:806:SER:O	1:A:808:LYS:O	2.36	0.44
1:A:575:LEU:HD23	1:A:595:SER:OG	2.17	0.44
1:A:898:ASN:C	1:A:900:GLY:H	2.20	0.44
1:A:767:LEU:O	1:A:771:LEU:HG	2.18	0.44
1:A:568:THR:O	1:A:571:ASP:HB2	2.18	0.44
1:A:766:GLN:HB2	1:A:766:GLN:HE21	1.68	0.44
1:A:564:LEU:O	1:A:1052:ARG:NH2	2.50	0.44
1:A:248:PHE:C	1:A:250:THR:H	2.20	0.43
1:A:954:ILE:HA	1:A:960:LEU:HA	2.00	0.43
1:A:144:SER:O	1:A:148:GLN:NE2	2.51	0.43
1:A:526:PRO:O	1:A:527:ILE:HG22	2.18	0.43
1:A:217:ASN:ND2	1:A:219:CYS:SG	2.92	0.43
1:A:248:PHE:O	1:A:251:LYS:N	2.49	0.43
1:A:702:GLU:HA	1:A:702:GLU:OE1	2.18	0.43
1:A:756:LYS:O	1:A:758:ASP:N	2.52	0.43
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.19	0.42
1:A:878:MET:C	1:A:879:ILE:HG13	2.40	0.42
1:A:660:LEU:O	1:A:664:VAL:HG23	2.19	0.42
1:A:381:VAL:HG21	1:A:404:PHE:CG	2.54	0.42
1:A:225:HIS:CE1	1:A:304:HIS:CD2	3.08	0.42
1:A:702:GLU:OE1	1:A:839:ARG:NH1	2.52	0.42
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:THR:HB	1:A:591:LYS:HE3	2.02	0.42
1:A:955:THR:HG1	1:A:959:ASN:H	1.66	0.42
1:A:463:TYR:CE2	1:A:501:LYS:HA	2.55	0.41
1:A:937:VAL:O	1:A:941:VAL:HG23	2.20	0.41
1:A:1089:HIS:O	1:A:1090:LEU:C	2.58	0.41
1:A:837:ASP:HB3	1:A:840:GLN:NE2	2.35	0.41
1:A:207:LEU:HD21	1:A:294:ARG:HG2	2.02	0.41
1:A:764:ILE:O	1:A:765:SER:C	2.59	0.41
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.94	0.41
1:A:579:ARG:HD2	1:A:610:LEU:HG	2.02	0.41
1:A:782:SER:O	1:A:783:PHE:HB3	2.21	0.41
1:A:411:ASN:O	1:A:411:ASN:CG	2.56	0.41
1:A:860:LEU:HD22	1:A:862:LEU:HD21	2.02	0.41
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.21	0.41
1:A:806:SER:HB2	1:A:810:PRO:HD3	2.03	0.41
1:A:997:THR:HG23	1:A:1001:LYS:HG3	2.03	0.40
1:A:764:ILE:O	1:A:768:LYS:HG2	2.21	0.40
1:A:312:ASP:HA	1:A:313:PRO:HD3	1.93	0.40
1:A:507:ASN:HA	1:A:508:PRO:HD2	1.98	0.40
1:A:682:LEU:HD22	1:A:686:LEU:HD11	2.02	0.40
1:A:391:GLN:OE1	1:A:633:CYS:HB2	2.21	0.40
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.57	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%)	744 (90%)	61 (7%)	22 (3%)	<b>6</b> <b>10</b>

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	ILE
1	A	561	THR
1	A	726	THR
1	A	776	ASN
1	A	1040	PRO
1	A	378	ASP
1	A	756	LYS
1	A	777	SER
1	A	899	THR
1	A	999	GLY
1	A	1000	LYS
1	A	1090	LEU
1	A	317	GLU
1	A	391	GLN
1	A	526	PRO
1	A	754	ALA
1	A	867	TYR
1	A	898	ASN
1	A	1044	SER
1	A	374	PRO
1	A	1084	PHE
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	757/864 (88%)	671 (89%)	86 (11%)	<b>7</b> <b>12</b>

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	168	VAL
1	A	204	SER
1	A	219	CYS
1	A	225	HIS

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Mol	Chain	Res	Type
1	A	226	ARG
1	A	229	THR
1	A	247	SER
1	A	252	MET
1	A	268	GLN
1	A	269	ASP
1	A	277	ARG
1	A	281	LEU
1	A	285	THR
1	A	287	ILE
1	A	291	GLN
1	A	307	LEU
1	A	309	THR
1	A	319	ARG
1	A	320	LYS
1	A	357	CYS
1	A	358	ASP
1	A	375	ARG
1	A	376	ASN
1	A	377	THR
1	A	378	ASP
1	A	379	LEU
1	A	406	GLU
1	A	418	ILE
1	A	487	ILE
1	A	520	LEU
1	A	525	HIS
1	A	550	GLN
1	A	565	ASN
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	646	GLN
1	A	662	GLN
1	A	682	LEU
1	A	688	ASN
1	A	701	SER
1	A	706	SER
1	A	717	LEU

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Mol	Chain	Res	Type
1	A	739	ILE
1	A	756	LYS
1	A	764	ILE
1	A	776	ASN
1	A	777	SER
1	A	807	LYS
1	A	811	LEU
1	A	825	ASN
1	A	838	LEU
1	A	841	ASP
1	A	843	LEU
1	A	845	LEU
1	A	862	LEU
1	A	865	LEU
1	A	871	SER
1	A	886	THR
1	A	896	VAL
1	A	912	LYS
1	A	913	GLU
1	A	915	SER
1	A	918	GLU
1	A	939	THR
1	A	967	HIS
1	A	982	ARG
1	A	1001	LYS
1	A	1002	THR
1	A	1011	ASP
1	A	1013	CYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1032	SER
1	A	1042	LEU
1	A	1044	SER
1	A	1046	GLU
1	A	1052	ARG
1	A	1056	THR
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 (20) 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
1	A	291	GLN
1	A	304	HIS
1	A	432	GLN
1	A	549	ASN
1	A	565	ASN
1	A	601	GLN
1	A	646	GLN
1	A	710	GLN
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	840	GLN
1	A	948	HIS
1	A	1007	GLN
1	A	1023	HIS
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	456	A	1201	-	20,23,23	1.54	5 (25%)	18,32,32	2.80	9 (50%)

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	456	A	1201	-	-	0/8/19/19	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	456	C8-C7	-3.14	1.36	1.42
2	A	1201	456	C8-S9	2.16	1.78	1.74
2	A	1201	456	C5-N4	2.26	1.40	1.36
2	A	1201	456	O20-C18	2.35	1.38	1.35
2	A	1201	456	C14-N11	2.44	1.42	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	456	C17-C18-N19	-6.19	119.03	123.11
2	A	1201	456	C15-C14-N19	-3.89	117.07	121.64
2	A	1201	456	C10-N11-C14	-3.64	110.22	117.60
2	A	1201	456	C12-N11-C14	-3.06	113.12	120.33
2	A	1201	456	O3-C2-C1	-2.10	118.23	122.06
2	A	1201	456	C13-C12-N11	2.66	118.53	110.32
2	A	1201	456	C1-C2-N4	3.30	119.87	115.02
2	A	1201	456	N19-C14-N11	3.91	121.01	116.61
2	A	1201	456	C21-O20-C18	4.01	122.64	117.38

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	456	1	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	843/966 (87%)	0.01	40 (4%) 32 25	40, 95, 166, 218	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	7.0
1	A	374	PRO	6.3
1	A	899	THR	6.3
1	A	323	TRP	6.1
1	A	1044	SER	6.1
1	A	248	PHE	4.8
1	A	1086	TRP	4.7
1	A	1088	LEU	4.7
1	A	322	GLU	4.6
1	A	212	TRP	4.4
1	A	825	ASN	4.4
1	A	901	ALA	4.4
1	A	987	LEU	4.3
1	A	377	THR	4.3
1	A	375	ARG	3.9
1	A	898	ASN	3.7
1	A	1091	VAL	3.7
1	A	254	LYS	3.6
1	A	404	PHE	3.5
1	A	221	PHE	3.4
1	A	991	PHE	3.3
1	A	378	ASP	3.1
1	A	403	PRO	3.1
1	A	235	VAL	3.0
1	A	544	ARG	3.0
1	A	902	PHE	2.9
1	A	215	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	249	PHE	2.9
1	A	1075	CYS	2.9
1	A	234	LYS	2.8
1	A	900	GLY	2.6
1	A	233	ILE	2.6
1	A	907	LEU	2.5
1	A	220	ILE	2.5
1	A	1089	HIS	2.4
1	A	272	LEU	2.3
1	A	895	THR	2.2
1	A	373	LEU	2.1
1	A	522	ASN	2.0
1	A	948	HIS	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(Å <sup>2</sup> )	Q<0.9
2	456	A	1201	21/21	0.97	0.14	-0.42	59,79,91,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.