



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:28 am BST

PDB ID : 3IBE  
Title : Crystal Structure of a Pyrazolopyrimidine Inhibitor Bound to PI3 Kinase Gamma  
Authors : Bard, J.; Svenson, K.  
Deposited on : 2009-07-15  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

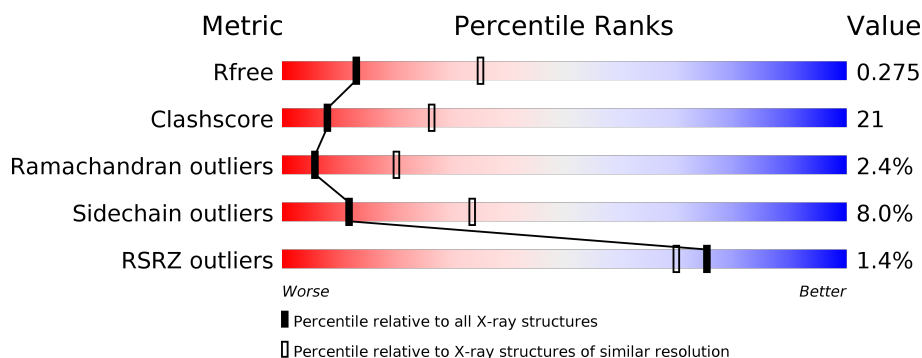
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	966	<div> <div></div> <div>51%</div> <div>34%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6622 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.

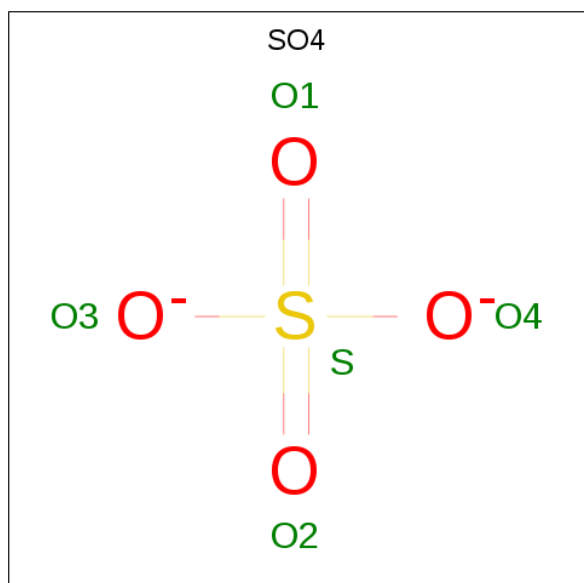
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	0	0
			6530	4195	1102	1199	34			

There are 8 discrepancies between the modelled and reference sequences:

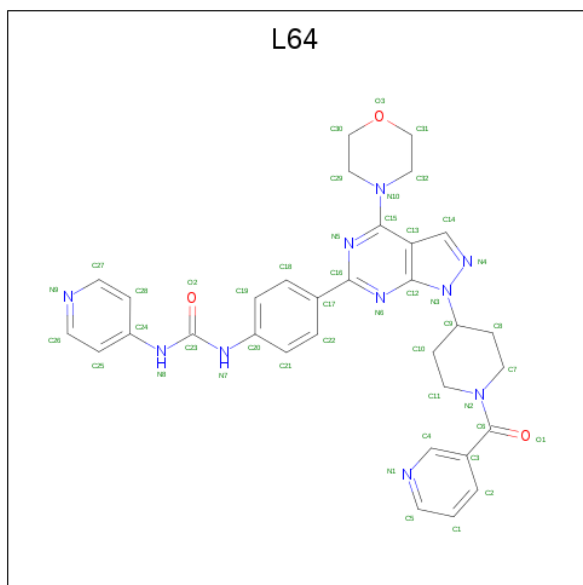
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	459	ARG	GLN	VARIANT	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1-(4-{4-morpholin-4-yl-1-[1-(pyridin-3-ylcarbonyl)piperidin-4-yl]-1H-pyrazolo[3,4-d]pyrimidin-6-yl}phenyl)-3-pyridin-4-ylurea (three-letter code: L64) (formula: C<sub>32</sub>H<sub>32</sub>N<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			45	32	10	3		

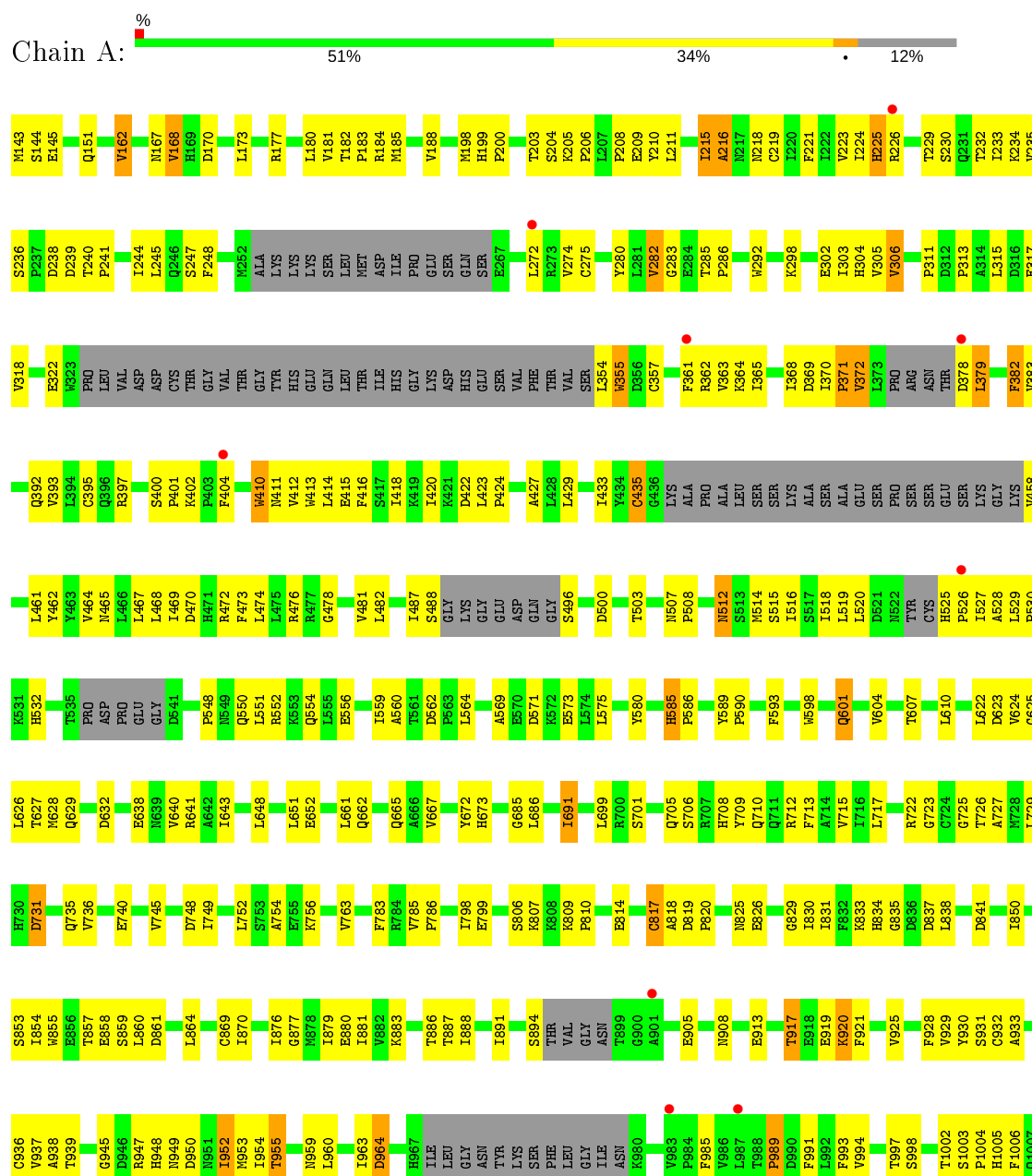
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		

### 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



K1008	F1009	Q1010	D1011	I1012	G1013	V1014	H1023	I1028	I1029	L1030	M1033	M1034	L1035	M1036	T1037	G1038	M1039	P1040	L1042	T1043	S1044	D1047	I1048	E1049	Y1050	T1051	R1052	T1056	M1060	Y1067	F1068	L1069	D1070	Q1071	I1072	K1078	G1079	H1080	T1081	N1085	W1086	F1087	L1088	H1089	L1090	V1091	L1092	GLY	I1E
LYS	GLN	GLY	GLU	LYS	HIS	SER	ALA	HIS	HIS	HIS	HIS	HIS	HIS	HIS	LYS	GLN	GLN	GLN	LYS	GLN	S1044	D1047	I1048	E1049	Y1050	T1051	R1052	T1056	M1060	Y1067	F1068	L1069	D1070	Q1071	I1072	K1078	G1079	H1080	T1081	N1085	W1086	F1087	L1088	H1089	L1090	V1091	L1092	GLY	I1E

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.16 Å   68.46 Å   106.90 Å 90.00°   94.80°   90.00°	Depositor
Resolution (Å)	44.71 – 2.80 44.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.1 (44.71-2.80) 83.2 (44.71-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.81 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.210   ,   0.277 0.201   ,   0.275	Depositor DCC
$R_{free}$ test set	1117 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.3	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	0.94	EDS
Total number of atoms	6622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: L64, SO4

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	0.56	0/6672	0.69	0/9081

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	6530	0	6206	272	0
2	A	5	0	0	0	0
3	A	45	0	32	7	0
4	A	42	0	0	1	0
All	All	6622	0	6238	274	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 21.

All (274) 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:180:LEU:O	1:A:183:PRO:HD2	1.83	0.79
1:A:953:MET:O	1:A:960:LEU:HD12	1.85	0.76
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.70	0.72
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.26	0.70
1:A:181:VAL:O	1:A:185:MET:HG3	1.94	0.68
1:A:627:THR:HG21	1:A:648:LEU:HD21	1.76	0.68
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.77	0.67
1:A:219:CYS:SG	1:A:234:LYS:HG2	2.35	0.66
1:A:397:ARG:HD2	1:A:415:GLU:O	1.95	0.66
1:A:731:ASP:O	1:A:735:GLN:HG3	1.95	0.66
1:A:936:CYS:SG	1:A:985:PHE:CD1	2.89	0.65
1:A:925:VAL:O	1:A:929:VAL:HG23	1.96	0.65
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.31	0.65
1:A:564:LEU:HD21	1:A:1048:ILE:HG22	1.77	0.65
1:A:514:MET:HG3	1:A:515:SER:N	2.11	0.65
1:A:833:LYS:O	1:A:876:ILE:HG13	1.96	0.65
1:A:370:ILE:HG12	1:A:371:PRO:O	1.97	0.65
1:A:378:ASP:O	1:A:379:LEU:HG	1.97	0.64
1:A:571:ASP:O	1:A:575:LEU:HD13	1.97	0.64
1:A:355:TRP:CE3	1:A:530:PRO:HG2	2.33	0.64
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.29	0.63
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.33	0.63
1:A:435:CYS:O	1:A:458:VAL:HA	1.98	0.63
1:A:933:ALA:O	1:A:937:VAL:HG23	1.98	0.62
1:A:368:ILE:HD13	1:A:514:MET:HE1	1.80	0.62
1:A:354:LEU:O	1:A:527:ILE:HD11	1.99	0.62
1:A:507:ASN:OD1	1:A:508:PRO:CD	2.48	0.62
1:A:224:ILE:O	1:A:230:SER:HA	1.99	0.62
1:A:888:ILE:O	1:A:891:ILE:HB	2.00	0.61
1:A:709:TYR:HB3	1:A:713:PHE:CE1	2.35	0.61
1:A:357:CYS:HB2	1:A:527:ILE:CD1	2.30	0.61
1:A:413:TRP:CH2	1:A:519:LEU:HD23	2.35	0.61
1:A:640:VAL:O	1:A:643:ILE:HG12	2.00	0.61
1:A:921:PHE:O	1:A:925:VAL:HG23	2.01	0.61
1:A:1081:THR:O	1:A:1085:ASN:OD1	2.18	0.61
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.83	0.60
1:A:464:VAL:HG22	1:A:465:ASN:H	1.65	0.60
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.37	0.60
1:A:1003:SER:HB2	1:A:1004:PRO:CD	2.31	0.60
1:A:955:THR:OG1	1:A:959:ASN:HB3	2.02	0.60
1:A:469:ILE:N	1:A:469:ILE:HD12	2.17	0.59
1:A:930:TYR:CE2	1:A:1012:ILE:HD13	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ILE:C	1:A:1050:TYR:N	2.55	0.59
1:A:461:LEU:C	1:A:462:TYR:CD2	2.75	0.59
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.36	0.59
1:A:726:THR:HA	1:A:729:LEU:HD12	1.84	0.59
1:A:952:ILE:HG22	1:A:953:MET:N	2.17	0.59
1:A:662:GLN:HG2	1:A:1030:LEU:CD2	2.32	0.58
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.84	0.58
1:A:953:MET:SD	1:A:963:ILE:HD13	2.43	0.58
1:A:302:GLU:O	1:A:304:HIS:CD2	2.55	0.58
1:A:936:CYS:HB3	1:A:985:PHE:CE1	2.39	0.58
1:A:952:ILE:CG2	1:A:960:LEU:HD11	2.33	0.58
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.85	0.58
1:A:1069:LEU:HA	1:A:1072:ILE:HG13	1.85	0.58
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.85	0.57
1:A:1048:ILE:C	1:A:1050:TYR:H	2.07	0.57
1:A:424:PRO:HG3	1:A:598:TRP:O	2.04	0.57
1:A:143:MET:C	1:A:145:GLU:H	2.07	0.57
1:A:1044:SER:HB3	1:A:1047:ASP:OD2	2.04	0.57
1:A:215:ILE:O	1:A:216:ALA:HB3	2.05	0.56
1:A:585:HIS:ND1	1:A:585:HIS:N	2.53	0.56
1:A:282:VAL:CG2	1:A:283:GLY:N	2.69	0.56
1:A:928:PHE:HZ	1:A:991:PHE:CD1	2.22	0.56
1:A:275:CYS:SG	1:A:306:VAL:HG12	2.46	0.56
1:A:928:PHE:O	1:A:932:CYS:HB3	2.06	0.56
1:A:357:CYS:HB2	1:A:527:ILE:HD12	1.87	0.56
1:A:624:VAL:O	1:A:628:MET:HG2	2.05	0.55
1:A:745:VAL:O	1:A:749:ILE:HG12	2.05	0.55
1:A:1035:LEU:O	1:A:1042:LEU:CB	2.53	0.55
1:A:225:HIS:N	1:A:225:HIS:CD2	2.74	0.55
1:A:236:SER:HB3	1:A:239:ASP:OD1	2.07	0.55
1:A:625:GLY:O	1:A:629:GLN:HG3	2.06	0.55
1:A:422:ASP:OD1	1:A:601:GLN:HB3	2.07	0.55
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.88	0.55
1:A:413:TRP:CZ2	1:A:519:LEU:HD23	2.41	0.55
1:A:831:ILE:O	1:A:831:ILE:HG22	2.05	0.54
1:A:952:ILE:HG21	1:A:960:LEU:HD11	1.90	0.54
1:A:685:GLY:HA2	1:A:691:ILE:CG2	2.38	0.54
1:A:853:SER:O	1:A:857:THR:HG23	2.07	0.54
1:A:831:ILE:HG13	1:A:881:ILE:HG13	1.90	0.54
1:A:913:GLU:O	1:A:913:GLU:HG2	2.08	0.54
1:A:280:TYR:HB3	1:A:282:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ILE:O	1:A:1050:TYR:N	2.40	0.53
1:A:1006:PHE:CE2	1:A:1010:GLN:CD	2.82	0.53
1:A:887:THR:HA	1:A:953:MET:HG2	1.89	0.53
1:A:317:GLU:HG2	1:A:318:VAL:N	2.24	0.53
1:A:837:ASP:O	3:A:1109:L64:C28	2.57	0.53
1:A:180:LEU:C	1:A:183:PRO:HD2	2.30	0.52
1:A:482:LEU:HB2	1:A:516:ILE:HG22	1.92	0.52
1:A:478:GLY:H	1:A:520:LEU:HB2	1.75	0.52
1:A:837:ASP:O	3:A:1109:L64:C27	2.57	0.52
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.39	0.52
1:A:208:PRO:HD2	1:A:211:LEU:HB2	1.90	0.52
1:A:1035:LEU:HB3	1:A:1042:LEU:HA	1.90	0.52
1:A:948:HIS:CD2	1:A:1086:TRP:HB2	2.45	0.52
1:A:507:ASN:OD1	1:A:508:PRO:HD2	2.10	0.52
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.43	0.51
1:A:274:VAL:HG21	1:A:292:TRP:NE1	2.26	0.51
1:A:496:SER:HB3	1:A:1043:THR:HB	1.93	0.51
1:A:879:ILE:HG22	1:A:880:GLU:N	2.25	0.51
1:A:361:PHE:HD2	1:A:416:PHE:HD1	1.58	0.51
1:A:876:ILE:O	1:A:876:ILE:HG23	2.10	0.51
1:A:365:ILE:O	1:A:365:ILE:HG22	2.09	0.50
1:A:274:VAL:CG2	1:A:292:TRP:CD1	2.94	0.50
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.93	0.50
1:A:559:ILE:O	1:A:559:ILE:HG22	2.12	0.50
1:A:580:TYR:CE2	1:A:610:LEU:CD1	2.94	0.50
1:A:315:LEU:O	1:A:727:ALA:HB2	2.10	0.50
1:A:1044:SER:HB3	1:A:1047:ASP:CG	2.32	0.50
1:A:205:LYS:HB3	1:A:206:PRO:HD2	1.93	0.50
1:A:182:THR:HB	1:A:183:PRO:HD3	1.93	0.49
1:A:469:ILE:CD1	1:A:469:ILE:N	2.74	0.49
1:A:667:VAL:HG12	1:A:667:VAL:O	2.11	0.49
1:A:1089:HIS:C	1:A:1091:VAL:H	2.15	0.49
1:A:1006:PHE:C	1:A:1006:PHE:CD2	2.85	0.49
1:A:302:GLU:O	1:A:304:HIS:N	2.46	0.49
1:A:238:ASP:HA	1:A:286:PRO:HB3	1.93	0.49
1:A:954:ILE:HA	1:A:959:ASN:O	2.12	0.49
1:A:809:LYS:N	1:A:810:PRO:HD3	2.28	0.49
1:A:736:VAL:O	1:A:740:GLU:HB2	2.13	0.49
1:A:936:CYS:SG	1:A:985:PHE:CE1	3.05	0.49
1:A:1056:THR:O	1:A:1056:THR:HG23	2.11	0.49
1:A:371:PRO:O	1:A:372:VAL:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ILE:N	1:A:952:ILE:CD1	2.75	0.49
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.76	0.48
1:A:1035:LEU:CD1	1:A:1048:ILE:HG12	2.42	0.48
1:A:952:ILE:CG2	1:A:953:MET:N	2.76	0.48
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.12	0.48
1:A:854:ILE:HG22	1:A:854:ILE:O	2.12	0.48
1:A:368:ILE:HD13	1:A:514:MET:SD	2.53	0.48
1:A:948:HIS:ND1	1:A:950:ASP:HB2	2.28	0.48
1:A:363:VAL:O	1:A:363:VAL:HG13	2.14	0.48
1:A:465:ASN:HB2	1:A:503:THR:O	2.13	0.48
1:A:550:GLN:O	1:A:554:GLN:HG3	2.14	0.48
1:A:837:ASP:O	3:A:1109:L64:H27	2.13	0.48
1:A:673:HIS:HA	1:A:712:ARG:HE	1.78	0.48
1:A:754:ALA:C	1:A:756:LYS:N	2.67	0.48
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.78	0.48
1:A:1023:HIS:N	1:A:1023:HIS:ND1	2.62	0.47
1:A:464:VAL:HG22	1:A:465:ASN:N	2.28	0.47
1:A:1067:TYR:O	1:A:1070:ASP:HB2	2.14	0.47
1:A:274:VAL:CG1	1:A:275:CYS:N	2.76	0.47
1:A:1078:LYS:O	1:A:1079:GLY:C	2.53	0.47
1:A:420:ILE:CG2	1:A:420:ILE:O	2.62	0.47
1:A:224:ILE:C	1:A:225:HIS:CD2	2.88	0.47
1:A:699:LEU:HD13	1:A:717:LEU:HB2	1.97	0.47
1:A:1078:LYS:O	1:A:1081:THR:HG23	2.13	0.47
1:A:361:PHE:HB2	1:A:420:ILE:HG13	1.97	0.47
1:A:184:ARG:HB2	1:A:184:ARG:HH11	1.79	0.47
1:A:725:GLY:O	1:A:729:LEU:HG	2.15	0.47
1:A:917:THR:OG1	1:A:919:GLU:HB3	2.15	0.47
1:A:379:LEU:HD13	1:A:435:CYS:SG	2.55	0.46
1:A:383:VAL:HG22	1:A:433:ILE:HG12	1.98	0.46
1:A:632:ASP:HB3	1:A:1033:MET:HE3	1.97	0.46
1:A:355:TRP:HE3	1:A:530:PRO:HG2	1.78	0.46
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.15	0.46
1:A:204:SER:HB2	1:A:652:GLU:OE2	2.15	0.46
1:A:604:VAL:O	1:A:607:THR:HB	2.15	0.46
1:A:298:LYS:HE3	1:A:861:ASP:OD2	2.16	0.46
1:A:686:LEU:CD2	1:A:723:GLY:C	2.83	0.46
1:A:382:PHE:HD1	1:A:382:PHE:H	1.64	0.46
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.80	0.46
1:A:472:ARG:O	1:A:473:PHE:HB2	2.16	0.46
1:A:368:ILE:C	1:A:368:ILE:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:HD13	1:A:514:MET:CE	2.46	0.46
1:A:748:ASP:O	1:A:752:LEU:HD13	2.16	0.46
1:A:1009:PHE:CD2	1:A:1009:PHE:C	2.89	0.46
1:A:274:VAL:CG2	1:A:292:TRP:NE1	2.79	0.46
1:A:240:THR:O	1:A:244:ILE:HG13	2.15	0.45
1:A:834:HIS:ND1	1:A:835:GLY:N	2.64	0.45
1:A:837:ASP:O	3:A:1109:L64:H28	2.17	0.45
1:A:1008:LYS:O	1:A:1011:ASP:HB2	2.17	0.45
1:A:223:VAL:HG12	1:A:225:HIS:NE2	2.31	0.45
1:A:569:ALA:O	1:A:573:GLU:HG3	2.16	0.45
1:A:825:ASN:O	1:A:826:GLU:C	2.53	0.45
1:A:997:THR:HG22	1:A:998:SER:N	2.31	0.45
1:A:552:ARG:O	1:A:556:GLU:HG3	2.16	0.45
1:A:917:THR:HG23	1:A:920:LYS:CD	2.47	0.45
1:A:306:VAL:O	1:A:306:VAL:HG22	2.17	0.45
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.99	0.45
1:A:936:CYS:SG	1:A:985:PHE:HD1	2.36	0.45
3:A:1109:L64:H19	3:A:1109:L64:O2	2.16	0.45
1:A:184:ARG:O	1:A:188:VAL:HG23	2.17	0.45
1:A:947:ARG:HG3	1:A:947:ARG:HH21	1.82	0.45
1:A:838:LEU:HD12	1:A:877:GLY:N	2.32	0.44
1:A:947:ARG:NH1	1:A:964:ASP:O	2.49	0.44
1:A:393:VAL:O	1:A:393:VAL:HG23	2.16	0.44
1:A:551:LEU:HA	1:A:551:LEU:HD23	1.75	0.44
1:A:686:LEU:HD22	1:A:723:GLY:O	2.17	0.44
1:A:525:HIS:N	1:A:526:PRO:CD	2.81	0.44
1:A:210:TYR:HE2	1:A:859:SER:HA	1.82	0.44
1:A:209:GLU:HB2	1:A:859:SER:HB3	2.00	0.44
1:A:372:VAL:HG12	1:A:372:VAL:O	2.17	0.44
1:A:496:SER:HA	1:A:1043:THR:O	2.17	0.44
1:A:955:THR:OG1	1:A:959:ASN:CB	2.65	0.44
1:A:210:TYR:HE2	1:A:860:LEU:N	2.16	0.44
1:A:661:LEU:O	1:A:665:GLN:HG2	2.17	0.44
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.48	0.44
1:A:931:SER:OG	1:A:932:CYS:N	2.50	0.44
1:A:550:GLN:O	1:A:550:GLN:HG3	2.17	0.44
1:A:167:ASN:C	1:A:168:VAL:CG1	2.85	0.43
1:A:514:MET:CG	1:A:515:SER:N	2.80	0.43
1:A:354:LEU:O	1:A:527:ILE:CG1	2.67	0.43
1:A:855:TRP:HZ3	1:A:864:LEU:HD11	1.82	0.43
1:A:210:TYR:CE2	1:A:860:LEU:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:O	1:A:379:LEU:CG	2.65	0.43
1:A:799:GLU:H	1:A:799:GLU:CD	2.22	0.43
1:A:1088:LEU:O	1:A:1091:VAL:HB	2.19	0.43
1:A:481:VAL:HA	1:A:516:ILE:O	2.18	0.43
1:A:830:ILE:HG22	1:A:831:ILE:N	2.33	0.43
1:A:939:THR:HB	1:A:945:GLY:HA2	2.00	0.43
1:A:931:SER:OG	1:A:960:LEU:HB3	2.19	0.43
1:A:215:ILE:O	1:A:216:ALA:CB	2.66	0.43
1:A:221:PHE:HD2	1:A:232:THR:CG2	2.32	0.43
1:A:170:ASP:C	1:A:170:ASP:OD1	2.57	0.43
1:A:589:TYR:O	1:A:593:PHE:CD1	2.72	0.43
1:A:855:TRP:O	1:A:860:LEU:O	2.36	0.43
1:A:908:ASN:OD1	1:A:994:VAL:HG22	2.17	0.43
1:A:401:PRO:O	1:A:402:LYS:HG3	2.19	0.43
1:A:925:VAL:O	1:A:925:VAL:HG12	2.17	0.43
1:A:1033:MET:O	1:A:1037:THR:HG23	2.19	0.42
1:A:857:THR:C	1:A:858:GLU:HG2	2.38	0.42
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.82	0.42
1:A:362:ARG:HG3	1:A:413:TRP:CZ3	2.54	0.42
1:A:829:GLY:O	1:A:881:ILE:HB	2.19	0.42
1:A:412:VAL:O	1:A:412:VAL:HG23	2.20	0.42
1:A:474:LEU:HD23	1:A:528:ALA:HB2	2.02	0.42
1:A:512:ASN:OD1	1:A:512:ASN:N	2.53	0.42
1:A:218:ASN:O	1:A:218:ASN:ND2	2.53	0.42
1:A:667:VAL:O	1:A:667:VAL:CG1	2.67	0.42
1:A:210:TYR:CE2	1:A:859:SER:HA	2.54	0.42
3:A:1109:L64:H29A	3:A:1109:L64:H14	2.01	0.42
1:A:143:MET:C	1:A:145:GLU:N	2.72	0.42
1:A:361:PHE:HD2	1:A:416:PHE:CD1	2.37	0.42
1:A:368:ILE:HG23	1:A:410:TRP:HZ3	1.83	0.42
1:A:470:ASP:CB	1:A:476:ARG:NH1	2.83	0.42
1:A:589:TYR:HB2	1:A:590:PRO:HD3	2.01	0.42
1:A:586:PRO:O	1:A:626:LEU:HD21	2.20	0.42
1:A:905:GLU:HG2	1:A:993:PHE:CE1	2.54	0.42
1:A:241:PRO:O	1:A:245:LEU:HD12	2.20	0.41
1:A:640:VAL:HG12	1:A:641:ARG:N	2.35	0.41
1:A:1089:HIS:O	1:A:1091:VAL:N	2.53	0.41
1:A:817:CYS:O	1:A:819:ASP:N	2.53	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.20	0.41
1:A:886:THR:HG23	1:A:887:THR:O	2.20	0.41
1:A:478:GLY:N	1:A:520:LEU:HB2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ILE:O	1:A:854:ILE:HG13	2.21	0.41
1:A:879:ILE:CG2	1:A:880:GLU:N	2.83	0.41
1:A:964:ASP:HA	3:A:1109:L64:C20	2.51	0.41
1:A:798:ILE:HG12	1:A:798:ILE:H	1.65	0.41
1:A:420:ILE:O	1:A:420:ILE:HG22	2.21	0.41
1:A:311:PRO:O	1:A:313:PRO:HD3	2.21	0.41
1:A:785:VAL:HA	1:A:786:PRO:HD3	1.91	0.41
1:A:917:THR:HG23	1:A:920:LYS:HD3	2.03	0.41
1:A:783:PHE:CD2	1:A:783:PHE:C	2.93	0.41
1:A:364:LYS:O	1:A:518:ILE:HA	2.21	0.41
1:A:1042:LEU:O	1:A:1043:THR:C	2.59	0.41
1:A:199:HIS:O	1:A:200:PRO:C	2.58	0.41
1:A:354:LEU:O	1:A:527:ILE:CD1	2.67	0.41
1:A:623:ASP:OD1	1:A:623:ASP:C	2.59	0.40
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.88	0.40
1:A:1089:HIS:C	1:A:1091:VAL:N	2.74	0.40
1:A:817:CYS:SG	1:A:819:ASP:HB3	2.62	0.40
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.90	0.40
1:A:883:LYS:HD3	1:A:883:LYS:HA	1.86	0.40
1:A:177:ARG:HG2	1:A:715:VAL:HG13	2.02	0.40
1:A:198:MET:O	1:A:199:HIS:C	2.60	0.40
1:A:1009:PHE:HE2	1:A:1072:ILE:HD13	1.86	0.40
1:A:1008:LYS:O	1:A:1011:ASP:CB	2.70	0.40
1:A:564:LEU:HD13	1:A:1028:ILE:CG2	2.52	0.40
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.85	0.40
1:A:560:ALA:HB2	4:A:86:HOH:O	2.22	0.40
1:A:622:LEU:HD21	1:A:651:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	828/966 (86%)	714 (86%)	94 (11%)	20 (2%)	6	20

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	ILE
1	A	371	PRO
1	A	216	ALA
1	A	372	VAL
1	A	638	GLU
1	A	691	ILE
1	A	964	ASP
1	A	1049	GLU
1	A	379	LEU
1	A	532	HIS
1	A	806	SER
1	A	818	ALA
1	A	1090	LEU
1	A	411	ASN
1	A	938	ALA
1	A	144	SER
1	A	162	VAL
1	A	989	PRO
1	A	215	ILE
1	A	1038	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	671/864 (78%)	617 (92%)	54 (8%)	12	34

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	VAL

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Mol	Chain	Res	Type
1	A	168	VAL
1	A	203	THR
1	A	225	HIS
1	A	226	ARG
1	A	229	THR
1	A	235	VAL
1	A	247	SER
1	A	282	VAL
1	A	285	THR
1	A	306	VAL
1	A	322	GLU
1	A	355	TRP
1	A	369	ASP
1	A	382	PHE
1	A	392	GLN
1	A	395	CYS
1	A	400	SER
1	A	404	PHE
1	A	410	TRP
1	A	418	ILE
1	A	435	CYS
1	A	487	ILE
1	A	488	SER
1	A	512	ASN
1	A	562	ASP
1	A	585	HIS
1	A	601	GLN
1	A	701	SER
1	A	705	GLN
1	A	731	ASP
1	A	763	VAL
1	A	807	LYS
1	A	814	GLU
1	A	817	CYS
1	A	841	ASP
1	A	869	CYS
1	A	870	ILE
1	A	894	SER
1	A	917	THR
1	A	920	LYS
1	A	949	ASN
1	A	952	ILE

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Mol	Chain	Res	Type
1	A	955	THR
1	A	989	PRO
1	A	1002	THR
1	A	1011	ASP
1	A	1023	HIS
1	A	1029	ILE
1	A	1039	MET
1	A	1049	GLU
1	A	1052	ARG
1	A	1060	ASN
1	A	1087	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

2 ligands are 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	SO4	A	1	-	4,4,4	0.15	0	6,6,6	0.23	0
3	L64	A	1109	-	49,51,51	0.88	4 (8%)	61,71,71	1.70	15 (24%)

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
3	L64	A	1109	-	-	2/24/46/46	0/7/7/7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1109	L64	C9-N3	-2.72	1.45	1.49
3	A	1109	L64	C15-N5	2.51	1.35	1.32
3	A	1109	L64	C3-C6	-2.33	1.46	1.50
3	A	1109	L64	C13-C12	-2.02	1.38	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1109	L64	C11-C10-C9	-4.68	106.78	110.44
3	A	1109	L64	C3-C6-N2	-4.64	112.82	118.72
3	A	1109	L64	C13-C15-N10	3.51	127.80	120.97
3	A	1109	L64	N8-C23-N7	-3.00	107.25	112.49
3	A	1109	L64	C8-C7-N2	-2.86	106.47	110.82
3	A	1109	L64	O1-C6-N2	2.80	126.96	122.34
3	A	1109	L64	C7-C8-C9	-2.77	108.27	110.44
3	A	1109	L64	C32-N10-C29	2.73	117.54	111.52
3	A	1109	L64	C16-N6-C12	-2.71	111.70	115.08
3	A	1109	L64	C13-C15-N5	-2.66	117.01	122.66
3	A	1109	L64	C1-C2-C3	-2.65	117.20	120.34
3	A	1109	L64	C10-C11-N2	-2.46	107.08	110.82
3	A	1109	L64	C14-C13-C12	-2.43	102.95	105.20
3	A	1109	L64	C2-C3-C4	2.26	120.19	117.63
3	A	1109	L64	C24-N8-C23	2.16	131.04	126.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

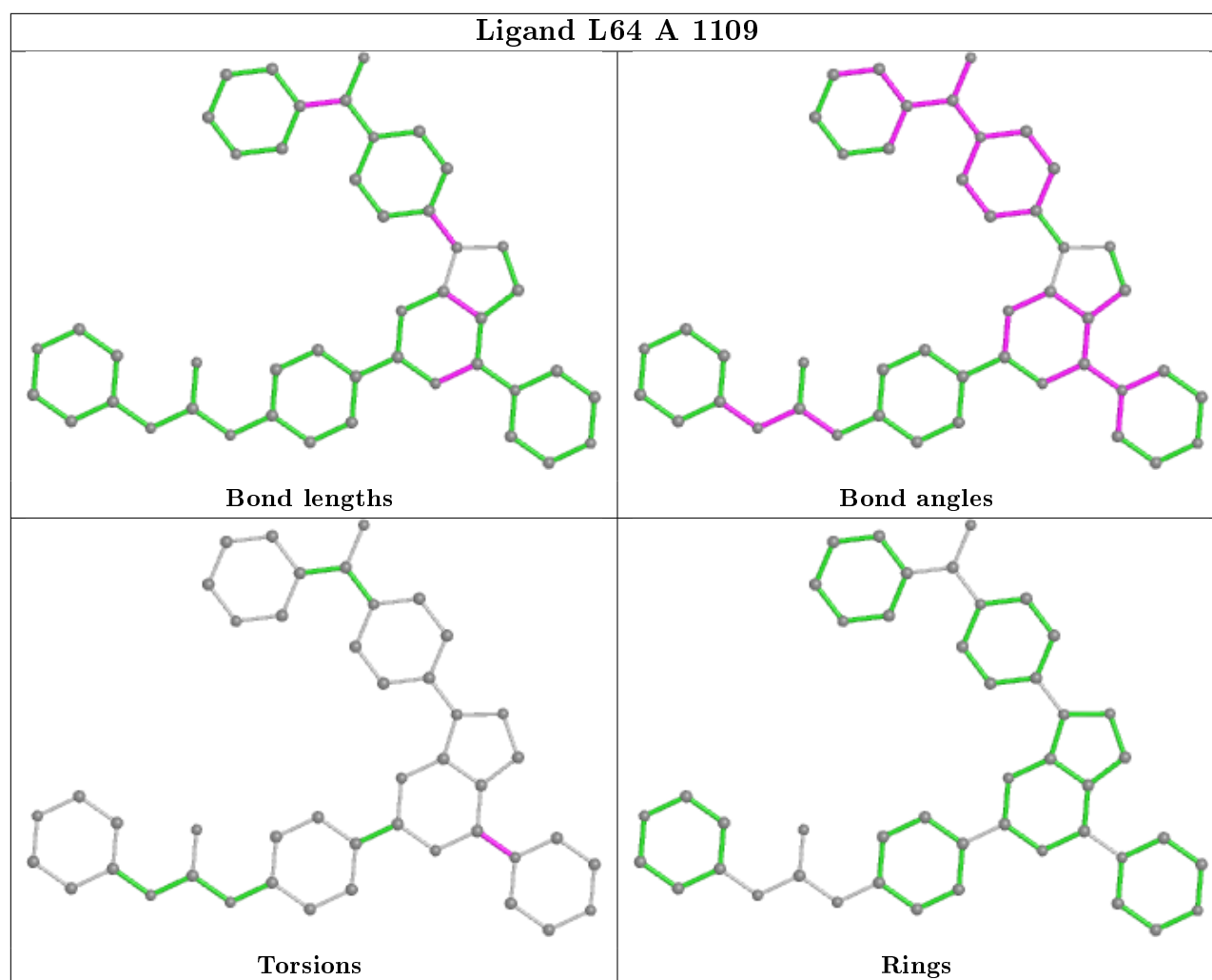
Mol	Chain	Res	Type	Atoms
3	A	1109	L64	N5-C15-N10-C29
3	A	1109	L64	C13-C15-N10-C29

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1109	L64	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	850/966 (87%)	-0.10	12 (1%) 75 70	34, 68, 115, 148	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	PHE	3.4
1	A	378	ASP	3.3
1	A	226	ARG	3.2
1	A	1086	TRP	2.9
1	A	901	ALA	2.9
1	A	361	PHE	2.7
1	A	272	LEU	2.3
1	A	983	VAL	2.3
1	A	1089	HIS	2.2
1	A	1087	PHE	2.2
1	A	526	PRO	2.2
1	A	987	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.

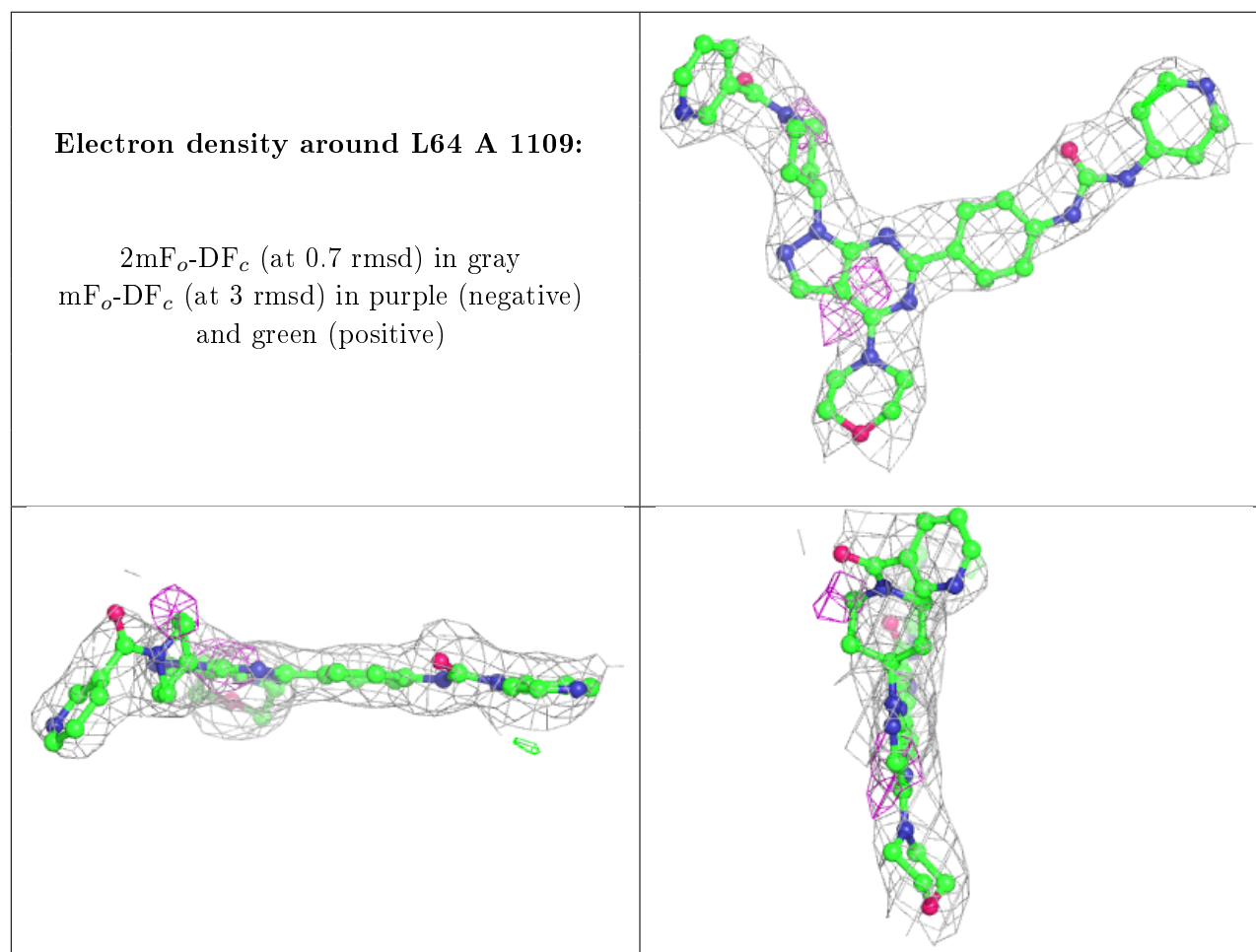
### 6.4 Ligands [i](#)

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. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	L64	A	1109	45/45	0.91	0.28	52,75,98,110	0
2	SO4	A	1	5/5	0.98	0.08	62,75,89,94	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.