



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:36 PM GMT

PDB ID : 4FJZ  
Title : Crystal structure of PI3K-gamma in complex with pyrrolo-pyridine inhibitor 63  
Authors : Whittington, D.A.; Tang, J.; Yakowec, P.  
Deposited on : 2012-06-12  
Resolution : 3.00 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

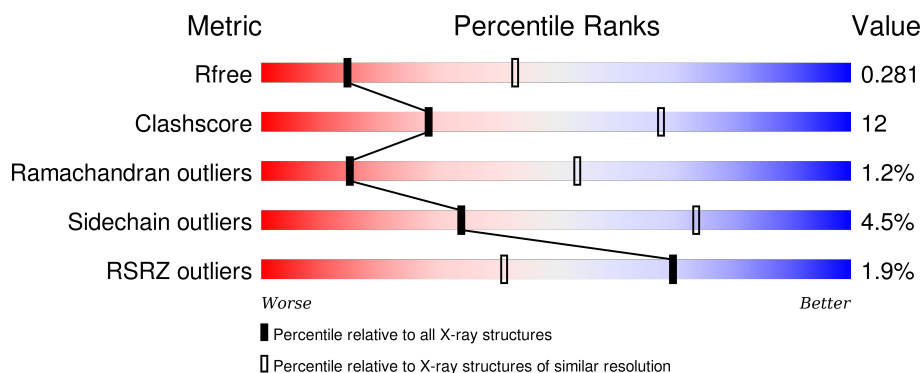
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	960	<div> <div>2%</div> <div>62%</div> <div>22%</div> <div>•</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1204	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6726 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 sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6658	4279	1134	1211	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLY	-	EXPRESSION TAG	UNP P48736

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



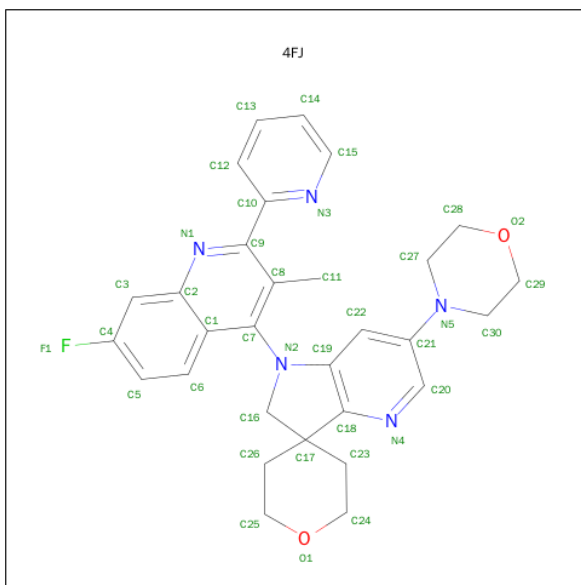
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 1'-[7-FLUORO-3-METHYL-2-(PYRIDIN-2-YL)QUINOLIN-4-YL]-6'-(MORPHOLIN-4-YL)-1',2,2',3,5,6-HEXAHYDROSPIRO[PYRAN-4,3'-PYRROLO[3,2-B]PYRIDINE] (three-letter code: 4FJ) (formula: C<sub>30</sub>H<sub>30</sub>FN<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	30	1	5	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.31Å 67.90Å 106.31Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-3.00) 97.6 (29.80-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.203 , 0.280 0.204 , 0.281	Depositor DCC
$R_{free}$ test set	1242 reflections (6.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 20266 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 4FJ

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	0.52	3/6796 (0.0%)	0.60	0/9187

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	TRP	CD2-CE2	5.35	1.47	1.41
1	A	1086	TRP	CD2-CE2	5.01	1.47	1.41
1	A	413	TRP	CD2-CE2	5.01	1.47	1.41

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	6658	0	6715	155	0
2	A	20	0	0	0	0
3	A	38	0	30	5	0
4	A	10	0	0	1	0
All	All	6726	0	6745	156	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 (156) 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:767:LEU:HD22	1:A:803:VAL:HG23	1.64	0.77
1:A:370:ILE:HD12	1:A:371:PRO:HD2	1.68	0.75
1:A:428:LEU:HD23	1:A:467:LEU:HD23	1.68	0.75
1:A:895:THR:HG22	1:A:896:VAL:HG23	1.69	0.73
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.19	0.73
1:A:576:TRP:O	1:A:579:ARG:HD3	1.89	0.72
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.72	0.71
1:A:726:THR:HA	1:A:729:LEU:HD12	1.73	0.70
1:A:941:VAL:HG21	1:A:1020:LEU:HD13	1.71	0.70
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.73	0.70
1:A:272:LEU:HD22	1:A:305:VAL:HG21	1.73	0.69
1:A:880:GLU:O	3:A:1205:4FJ:H17	1.94	0.68
1:A:198:MET:CE	1:A:282:VAL:HG21	2.25	0.66
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.31	0.65
1:A:953:MET:SD	3:A:1205:4FJ:H20	2.38	0.62
1:A:365:ILE:HD13	1:A:518:ILE:HG22	1.81	0.62
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.81	0.61
1:A:223:VAL:HG22	1:A:232:THR:HG23	1.82	0.61
1:A:1009:PHE:HE2	1:A:1072:ILE:HD13	1.66	0.60
1:A:1020:LEU:HD22	1:A:1027:LEU:HD11	1.83	0.60
1:A:937:VAL:O	1:A:941:VAL:HG23	2.01	0.59
1:A:158:ILE:HG23	1:A:703:ILE:HD13	1.86	0.58
1:A:952:ILE:CD1	1:A:986:VAL:HG11	2.34	0.58
1:A:745:VAL:O	1:A:749:ILE:HD13	2.04	0.58
1:A:395:CYS:SG	1:A:417:SER:OG	2.61	0.58
1:A:811:LEU:HB3	1:A:813:LEU:HD21	1.85	0.58
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.85	0.58
1:A:798:ILE:H	1:A:798:ILE:HD12	1.69	0.57
1:A:779:LEU:HD23	1:A:780:PRO:O	2.04	0.57
1:A:379:LEU:HD22	1:A:436:GLY:O	2.04	0.57
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.86	0.57
1:A:869:CYS:O	1:A:870:ILE:HD13	2.04	0.57
1:A:162:VAL:CG1	1:A:177:ARG:HD2	2.34	0.57
1:A:895:THR:HG22	1:A:896:VAL:CG2	2.36	0.56
1:A:804:MET:HE2	1:A:810:PRO:HG2	1.88	0.56
1:A:925:VAL:HG13	1:A:994:VAL:HG12	1.87	0.56
1:A:475:LEU:HD23	1:A:476:ARG:H	1.71	0.56
1:A:980:LYS:HE3	1:A:1088:LEU:HD11	1.87	0.56
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.87	0.55
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:LEU:HD23	1:A:1021:ARG:HD3	1.88	0.55
1:A:937:VAL:HG21	1:A:1016:ALA:HB3	1.89	0.55
1:A:1007:GLN:O	1:A:1011:ASP:N	2.38	0.55
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.46	0.54
1:A:732:PHE:O	1:A:736:VAL:HG23	2.07	0.54
1:A:833:LYS:HG3	3:A:1205:4FJ:H12	1.88	0.54
1:A:742:LEU:HD22	1:A:813:LEU:CD1	2.38	0.54
1:A:705:GLN:NE2	1:A:837:ASP:OD1	2.41	0.54
1:A:665:GLN:NE2	1:A:702:GLU:OE2	2.32	0.53
1:A:804:MET:CE	1:A:806:SER:HB3	2.39	0.53
1:A:475:LEU:HD23	1:A:476:ARG:N	2.24	0.53
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.38	0.53
1:A:941:VAL:HG21	1:A:1020:LEU:CD1	2.39	0.53
1:A:498:ASN:HD22	1:A:499:ALA:N	2.07	0.53
1:A:370:ILE:HD12	1:A:371:PRO:CD	2.38	0.52
1:A:631:LEU:HD21	1:A:644:ALA:HB3	1.90	0.52
1:A:208:PRO:HG2	1:A:211:LEU:HD12	1.90	0.52
1:A:162:VAL:HG13	1:A:177:ARG:HD2	1.91	0.52
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.91	0.51
1:A:176:THR:HG23	1:A:674:ASP:CB	2.39	0.51
1:A:272:LEU:HB3	1:A:305:VAL:HG21	1.93	0.51
1:A:586:PRO:O	1:A:626:LEU:HD21	2.11	0.51
1:A:785:VAL:HG23	1:A:791:LEU:O	2.11	0.51
1:A:583:LEU:HD13	1:A:610:LEU:HG	1.93	0.51
1:A:988:THR:HG21	1:A:1083:GLN:HG3	1.93	0.50
1:A:602:GLU:O	1:A:605:ALA:HB3	2.12	0.50
1:A:952:ILE:HD12	1:A:986:VAL:HG11	1.94	0.50
1:A:761:SER:HA	1:A:764:ILE:HD12	1.93	0.50
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.11	0.50
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.93	0.50
1:A:880:GLU:O	3:A:1205:4FJ:C28	2.59	0.49
1:A:1031:PHE:CE2	1:A:1035:LEU:HD11	2.48	0.49
1:A:579:ARG:HG2	1:A:610:LEU:HD22	1.96	0.48
1:A:632:ASP:C	1:A:632:ASP:OD1	2.52	0.48
1:A:559:ILE:O	1:A:559:ILE:HG22	2.13	0.48
1:A:219:CYS:HA	1:A:235:VAL:O	2.14	0.48
1:A:989:PRO:O	1:A:993:PHE:N	2.41	0.48
1:A:855:TRP:CD2	1:A:862:LEU:HD13	2.48	0.48
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.28	0.48
1:A:547:MET:HE2	1:A:552:ARG:N	2.29	0.48
1:A:387:ILE:HD12	1:A:468:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.96	0.48
1:A:184:ARG:O	1:A:188:VAL:HG23	2.14	0.48
1:A:1033:MET:O	1:A:1037:THR:HG23	2.14	0.48
1:A:947:ARG:NH2	1:A:964:ASP:O	2.47	0.48
1:A:1007:GLN:HA	1:A:1010:GLN:HE21	1.79	0.47
1:A:863:CYS:SG	1:A:930:TYR:HB3	2.54	0.47
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.41	0.47
1:A:743:GLN:NE2	1:A:876:ILE:HG23	2.29	0.47
1:A:1050:TYR:CE2	1:A:1054:ALA:HB2	2.50	0.47
1:A:862:LEU:HD21	1:A:1016:ALA:HB2	1.96	0.47
1:A:387:ILE:HD12	1:A:468:LEU:CD1	2.44	0.47
1:A:357:CYS:H	1:A:527:ILE:HD11	1.80	0.47
1:A:686:LEU:HD23	1:A:720:TYR:CE1	2.50	0.46
1:A:545:ALA:HB1	1:A:584:LYS:NZ	2.31	0.46
1:A:742:LEU:HD22	1:A:813:LEU:HD11	1.97	0.46
1:A:233:ILE:HD13	1:A:247:SER:OG	2.15	0.46
1:A:182:THR:HB	1:A:183:PRO:CD	2.45	0.46
1:A:876:ILE:O	1:A:876:ILE:HG23	2.16	0.46
1:A:665:GLN:HE22	1:A:702:GLU:CD	2.15	0.45
1:A:805:ALA:HB3	4:A:1307:HOH:O	2.16	0.45
1:A:804:MET:HE2	1:A:810:PRO:CG	2.46	0.45
1:A:997:THR:HG22	1:A:998:SER:N	2.32	0.45
1:A:487:ILE:HG22	1:A:488:SER:H	1.81	0.45
1:A:235:VAL:HG12	1:A:239:ASP:HB2	1.98	0.45
1:A:814:GLU:OE2	1:A:827:THR:OG1	2.32	0.45
1:A:272:LEU:CD2	1:A:305:VAL:HG11	2.47	0.45
1:A:935:TYR:O	1:A:939:THR:HG23	2.16	0.45
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.99	0.44
1:A:576:TRP:CZ3	1:A:596:VAL:HG22	2.52	0.44
1:A:948:HIS:ND1	1:A:950:ASP:OD1	2.50	0.44
3:A:1205:4FJ:H8	3:A:1205:4FJ:H19	1.82	0.44
1:A:1035:LEU:O	1:A:1043:THR:HG22	2.18	0.44
1:A:853:SER:O	1:A:857:THR:HG23	2.18	0.44
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.52	0.44
1:A:803:VAL:HG22	1:A:811:LEU:HD23	1.99	0.43
1:A:305:VAL:HG22	1:A:306:VAL:H	1.84	0.43
1:A:905:GLU:HA	1:A:993:PHE:CE2	2.53	0.43
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.49	0.43
1:A:949:ASN:H	1:A:949:ASN:HD22	1.66	0.43
1:A:891:ILE:O	1:A:906:VAL:HG11	2.19	0.43
1:A:182:THR:HB	1:A:183:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:HD12	1:A:516:ILE:HD11	2.00	0.43
1:A:162:VAL:HG12	1:A:177:ARG:NH1	2.33	0.43
1:A:366:ARG:NH1	1:A:519:LEU:HD22	2.33	0.43
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.91	0.43
1:A:739:ILE:C	1:A:739:ILE:HD12	2.39	0.43
1:A:305:VAL:HG13	1:A:306:VAL:N	2.34	0.42
1:A:467:LEU:O	1:A:476:ARG:HD2	2.19	0.42
1:A:208:PRO:CG	1:A:211:LEU:HD12	2.50	0.42
1:A:287:ILE:HD12	1:A:288:LYS:N	2.34	0.42
1:A:811:LEU:HB3	1:A:813:LEU:CD2	2.48	0.42
1:A:862:LEU:N	1:A:862:LEU:HD12	2.34	0.42
1:A:997:THR:HG22	1:A:998:SER:H	1.83	0.42
1:A:640:VAL:O	1:A:643:ILE:HG12	2.19	0.42
1:A:663:LEU:HA	1:A:663:LEU:HD23	1.94	0.42
1:A:273:ARG:H	1:A:305:VAL:HG22	1.85	0.42
1:A:371:PRO:HG2	1:A:511:GLU:O	2.19	0.42
1:A:224:ILE:HA	1:A:305:VAL:HG12	2.02	0.41
1:A:198:MET:HE1	1:A:282:VAL:HG21	2.02	0.41
1:A:745:VAL:CG2	1:A:774:LEU:HD12	2.50	0.41
1:A:788:ASP:OD2	1:A:791:LEU:HD12	2.20	0.41
1:A:702:GLU:O	1:A:706:SER:HB3	2.20	0.41
1:A:759:VAL:HG12	1:A:764:ILE:HG13	2.01	0.41
1:A:271:VAL:HG13	1:A:282:VAL:CG1	2.50	0.41
1:A:865:LEU:HD22	1:A:882:VAL:HG21	2.03	0.41
1:A:775:GLN:HE22	1:A:796:LEU:H	1.68	0.41
1:A:702:GLU:OE1	1:A:839:ARG:NH2	2.54	0.41
1:A:1014:VAL:HG11	1:A:1065:LYS:CG	2.51	0.41
1:A:795:ALA:HB3	1:A:816:LYS:HB2	2.03	0.41
1:A:368:ILE:HG21	1:A:433:ILE:HD11	2.03	0.40
1:A:728:MET:HA	1:A:731:ASP:HB2	2.03	0.40
1:A:674:ASP:OD1	1:A:679:ARG:NE	2.54	0.40
1:A:614:ARG:CZ	1:A:643:ILE:HG22	2.52	0.40
1:A:775:GLN:OE1	1:A:798:ILE:HD11	2.21	0.40
1:A:937:VAL:HG12	1:A:1020:LEU:HD12	2.04	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	800/960 (83%)	724 (90%)	66 (8%)	10 (1%)	15	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	916	PRO
1	A	1079	GLY
1	A	217	ASN
1	A	778	GLN
1	A	761	SER
1	A	777	SER
1	A	964	ASP
1	A	319	ARG
1	A	999	GLY
1	A	1040	PRO

### 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	739/857 (86%)	706 (96%)	33 (4%)	34	74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	LYS

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Mol	Chain	Res	Type
1	A	232	THR
1	A	235	VAL
1	A	240	THR
1	A	305	VAL
1	A	317	GLU
1	A	391	GLN
1	A	395	CYS
1	A	488	SER
1	A	498	ASN
1	A	515	SER
1	A	522	ASN
1	A	707	ARG
1	A	731	ASP
1	A	739	ILE
1	A	758	ASP
1	A	769	GLN
1	A	796	LEU
1	A	804	MET
1	A	823	LEU
1	A	833	LYS
1	A	847	ILE
1	A	863	CYS
1	A	865	LEU
1	A	869	CYS
1	A	906	VAL
1	A	917	THR
1	A	949	ASN
1	A	959	ASN
1	A	967	HIS
1	A	982	ARG
1	A	1002	THR
1	A	1029	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	391	GLN
1	A	486	GLN
1	A	498	ASN
1	A	619	GLN
1	A	734	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	743	GLN
1	A	773	ASN
1	A	846	GLN
1	A	922	GLN
1	A	959	ASN
1	A	1010	GLN
1	A	1023	HIS

### 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 ⓘ

5 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	1201	-	4,4,4	0.44	0	6,6,6	0.23	0
2	SO4	A	1202	-	4,4,4	0.43	0	6,6,6	0.13	0
2	SO4	A	1203	-	4,4,4	0.38	0	6,6,6	0.25	0
2	SO4	A	1204	-	4,4,4	0.48	0	6,6,6	0.10	0
3	4FJ	A	1205	-	43,44,44	2.12	5 (11%)	56,65,65	1.88	20 (35%)

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	SO4	A	1201	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1202	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1203	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1204	-	-	0/0/0/0	0/0/0/0
3	4FJ	A	1205	-	-	0/12/45/45	0/7/7/7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1205	4FJ	C7-N2	-9.60	1.35	1.44
3	A	1205	4FJ	C9-C10	-7.76	1.40	1.49
3	A	1205	4FJ	C19-N2	-2.39	1.34	1.38
3	A	1205	4FJ	C7-C1	-2.28	1.40	1.43
3	A	1205	4FJ	C3-C4	2.07	1.39	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1205	4FJ	O1-C25-C26	-4.92	106.84	111.57
3	A	1205	4FJ	C5-C4-C3	-3.28	119.70	123.51
3	A	1205	4FJ	C8-C9-N1	-3.13	120.65	123.19
3	A	1205	4FJ	C25-C26-C17	-2.89	108.90	111.99
3	A	1205	4FJ	C10-C9-C8	-2.49	121.71	124.17
3	A	1205	4FJ	C6-C1-C7	-2.36	120.32	124.77
3	A	1205	4FJ	C19-C18-N4	-2.34	121.69	125.18
3	A	1205	4FJ	C22-C19-C18	-2.30	117.65	120.08
3	A	1205	4FJ	C1-C2-N1	-2.28	120.67	122.90
3	A	1205	4FJ	C9-N1-C2	2.05	121.13	117.08
3	A	1205	4FJ	C8-C7-N2	2.10	121.58	119.02
3	A	1205	4FJ	C7-C1-C2	2.15	120.30	115.93
3	A	1205	4FJ	C22-C19-N2	2.26	131.50	128.79
3	A	1205	4FJ	C1-C7-N2	2.33	120.66	117.64
3	A	1205	4FJ	C26-C17-C23	2.37	111.17	108.90
3	A	1205	4FJ	C16-N2-C19	2.60	111.99	109.28
3	A	1205	4FJ	C15-N3-C10	2.98	121.31	117.20
3	A	1205	4FJ	C20-N4-C18	3.10	121.27	117.81
3	A	1205	4FJ	C27-N5-C30	3.24	118.39	111.59
3	A	1205	4FJ	C9-C10-N3	3.70	121.52	116.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1205	4FJ	5	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 [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	822/960 (85%)	-0.25	16 (1%) 70 41	48, 85, 133, 155	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1042	LEU	3.6
1	A	999	GLY	3.6
1	A	228	THR	3.3
1	A	1000	LYS	3.2
1	A	777	SER	2.7
1	A	998	SER	2.6
1	A	270	PHE	2.5
1	A	356	ASP	2.2
1	A	148	GLN	2.2
1	A	1001	LYS	2.2
1	A	545	ALA	2.2
1	A	531	LYS	2.1
1	A	986	VAL	2.0
1	A	1041	GLN	2.0
1	A	496	SER	2.0
1	A	753	SER	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	SO4	A	1204	5/5	0.92	0.27	5.09	107,110,116,119	0
2	SO4	A	1202	5/5	0.92	0.29	1.48	117,124,128,130	0
3	4FJ	A	1205	38/38	0.91	0.21	0.15	77,99,111,114	0
2	SO4	A	1203	5/5	0.84	0.21	-0.45	149,152,155,158	0
2	SO4	A	1201	5/5	0.92	0.17	-0.59	93,95,101,109	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.