



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:27 PM GMT

PDB ID : 4EZK  
Title : Potent and Selective Inhibitors of PI3K-delta: Obtaining Isoform Selectivity from the Affinity Pocket and Tryptophan Shelf  
Authors : Murray, J.M.  
Deposited on : 2012-05-02  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

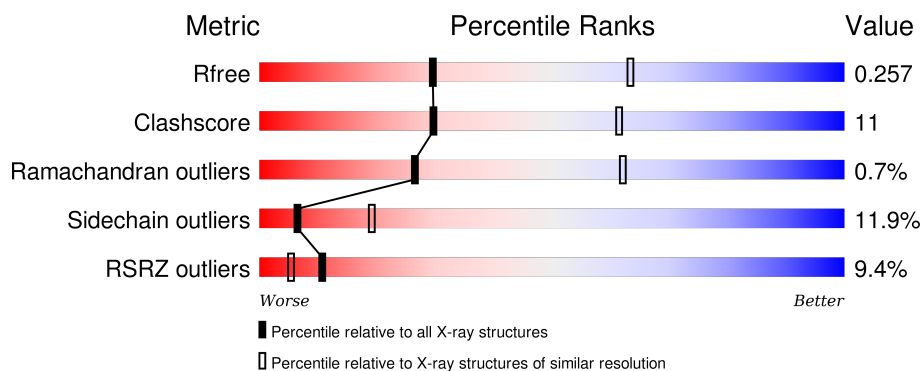
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6866 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.

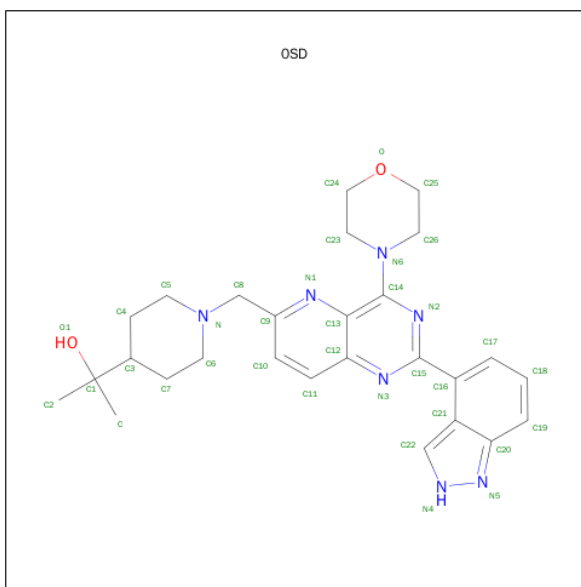
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	0	0
			6818	4375	1164	1244	35			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	802	THR	LYS	ENGINEERED MUTATION	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 2-(1-{[2-(2H-INDAZOL-4-YL)-4-(MORPHOLIN-4-YL)PYRIDO[3,2-D]PYRIMIDIN-6-YL]METHYL}PIPERIDIN-4-YL)PROPAN-2-OL (three-letter code: OSD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	1	0
			36	27	7	2		

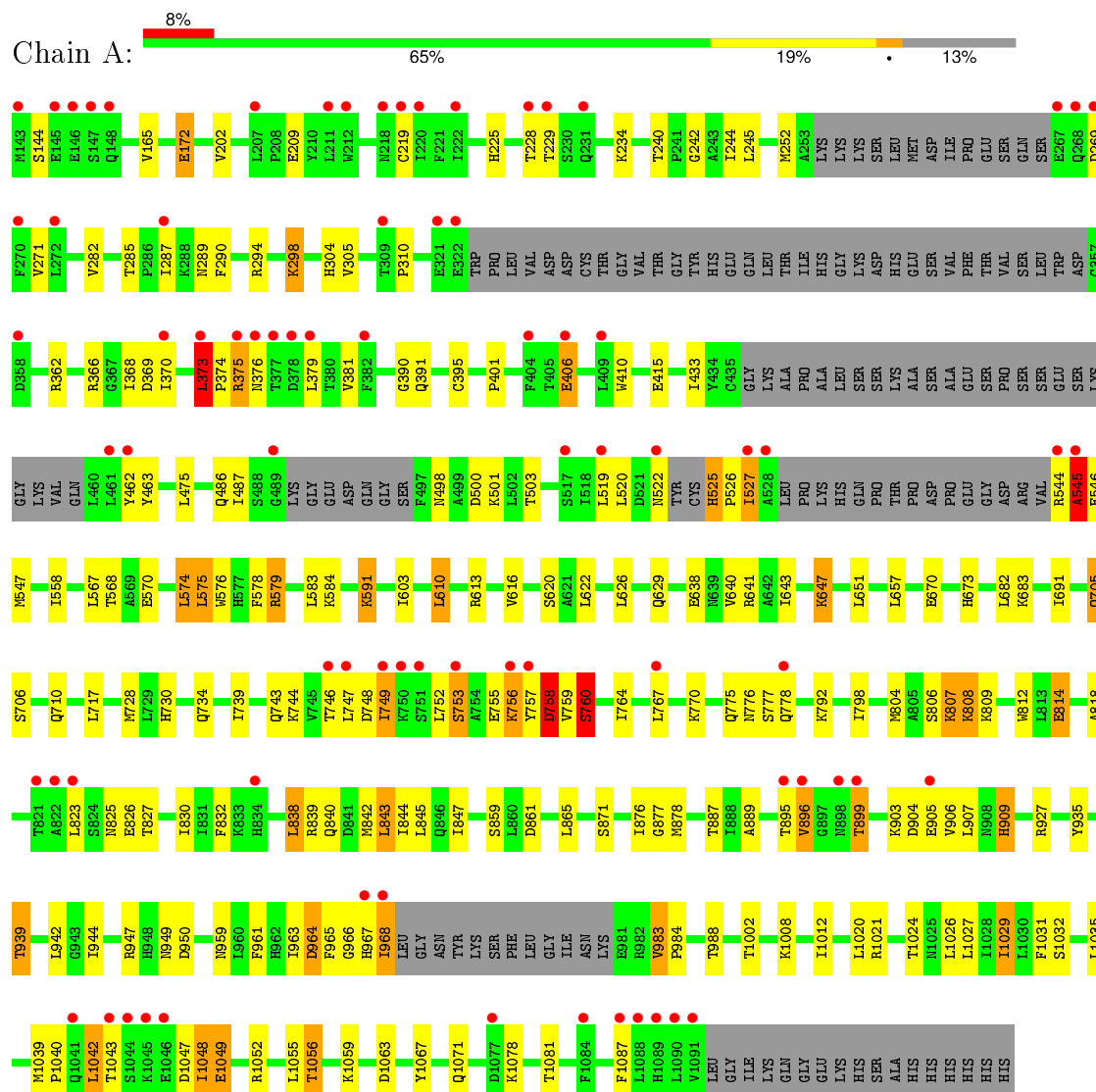
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		

### 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 errors 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, $\alpha$ , $\beta$ , $\gamma$	140.73Å 67.19Å 106.02Å 90.00° 96.76° 90.00°	Depositor
Resolution (Å)	34.39 – 2.80 34.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (34.39-2.80) 95.5 (34.39-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1066)	Depositor
R, $R_{free}$	0.243 , 0.253 0.252 , 0.257	Depositor DCC
$R_{free}$ test set	1202 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 90.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 23300 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0SD

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	0.44	1/6964 (0.0%)	0.66	6/9422 (0.1%)

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	1040	PRO	N-CD	5.25	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	545	ALA	N-CA-C	9.05	135.43	111.00
1	A	252	MET	CB-CA-C	7.43	125.26	110.40
1	A	964	ASP	N-CA-C	7.17	130.35	111.00
1	A	410	TRP	CB-CA-C	6.26	122.92	110.40
1	A	1039	MET	C-N-CD	5.42	139.78	128.40
1	A	410	TRP	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	ALA	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	6818	0	6848	148	0
2	A	36	0	33	7	0
3	A	12	0	0	0	0
All	All	6866	0	6881	154	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 11.

All (154) 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:525:HIS:HB3	1:A:526:PRO:HD3	1.26	1.10
1:A:576:TRP:O	1:A:579:ARG:HG2	1.53	1.06
1:A:757:TYR:CB	1:A:758:ASP:HB2	1.90	1.01
2:A:4000:OSD:H21	2:A:4000:OSD:H13	1.45	0.98
1:A:525:HIS:CB	1:A:526:PRO:HD3	1.91	0.97
1:A:757:TYR:HB2	1:A:758:ASP:HB2	1.51	0.90
2:A:4000:OSD:C10	2:A:4000:OSD:H13	2.02	0.89
1:A:743:GLN:HE21	1:A:876:ILE:CD1	1.87	0.88
1:A:375:ARG:HD2	1:A:376:ASN:H	1.37	0.88
2:A:4000:OSD:H34	2:A:4000:OSD:N1	1.89	0.86
1:A:743:GLN:NE2	1:A:876:ILE:CD1	2.40	0.85
1:A:759:VAL:HA	1:A:760:SER:CB	2.06	0.84
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.60	0.83
1:A:370:ILE:O	1:A:406:GLU:HB3	1.78	0.82
2:A:4000:OSD:C5	2:A:4000:OSD:H21	2.10	0.80
1:A:749:ILE:O	1:A:753:SER:HB2	1.82	0.79
1:A:759:VAL:HA	1:A:760:SER:HB2	1.64	0.78
1:A:375:ARG:CD	1:A:376:ASN:H	1.97	0.78
1:A:753:SER:CB	1:A:809:LYS:HG3	2.13	0.77
1:A:743:GLN:NE2	1:A:876:ILE:HD12	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ARG:HG2	1:A:579:ARG:HH11	1.54	0.73
1:A:228:THR:O	1:A:229:THR:HG23	1.90	0.72
1:A:757:TYR:CA	1:A:758:ASP:HB2	2.20	0.72
1:A:375:ARG:HD2	1:A:376:ASN:N	2.05	0.72
1:A:947:ARG:NH2	1:A:963:ILE:O	2.23	0.71
1:A:525:HIS:CB	1:A:526:PRO:CD	2.67	0.70
1:A:840:GLN:OE1	1:A:968:ILE:C	2.29	0.70
1:A:743:GLN:HE21	1:A:876:ILE:HD11	1.57	0.69
1:A:527:ILE:O	1:A:527:ILE:HG22	1.92	0.68
1:A:373:LEU:CD2	1:A:406:GLU:HG3	2.23	0.68
1:A:748:ASP:O	1:A:752:LEU:HD23	1.94	0.68
2:A:4000:OSD:C5	2:A:4000:OSD:C10	2.71	0.68
1:A:743:GLN:HG3	1:A:876:ILE:HD13	1.75	0.67
1:A:777:SER:HB2	1:A:778:GLN:HG2	1.76	0.66
1:A:944:ILE:HD12	1:A:965:PHE:CE1	2.32	0.64
1:A:579:ARG:CG	1:A:579:ARG:HH11	2.12	0.63
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.81	0.61
1:A:544:ARG:HG2	1:A:545:ALA:H	1.65	0.61
1:A:544:ARG:O	1:A:545:ALA:HB3	2.00	0.60
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.83	0.60
1:A:574:LEU:HD22	1:A:578:PHE:CD2	2.37	0.59
1:A:575:LEU:HD21	1:A:591:LYS:HB3	1.84	0.59
1:A:1021:ARG:NE	1:A:1056:THR:HG22	2.19	0.58
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.67	0.58
1:A:807:LYS:H	1:A:807:LYS:HE2	1.67	0.58
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.17	0.57
1:A:968:ILE:H	1:A:968:ILE:HD13	1.69	0.57
1:A:228:THR:O	1:A:229:THR:CG2	2.51	0.57
1:A:228:THR:HG22	1:A:228:THR:O	2.04	0.57
1:A:843:LEU:O	1:A:847:ILE:HD12	2.04	0.57
1:A:777:SER:OG	1:A:778:GLN:HG3	2.05	0.57
1:A:759:VAL:HA	1:A:760:SER:HB3	1.87	0.56
1:A:271:VAL:HG23	1:A:310:PRO:HG3	1.87	0.56
1:A:743:GLN:HG3	1:A:876:ILE:CD1	2.36	0.55
1:A:757:TYR:CA	1:A:758:ASP:CB	2.85	0.54
2:A:4000:OSD:C26	2:A:4000:OSD:N1	2.68	0.54
1:A:777:SER:HB2	1:A:778:GLN:CG	2.37	0.54
1:A:756:LYS:HE3	1:A:807:LYS:HD3	1.88	0.54
1:A:887:THR:HG22	1:A:889:ALA:H	1.72	0.54
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.88	0.54
1:A:840:GLN:O	1:A:844:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:GLN:CG	1:A:876:ILE:HD13	2.37	0.54
1:A:228:THR:C	1:A:229:THR:HG23	2.29	0.54
1:A:568:THR:HG22	1:A:570:GLU:N	2.23	0.53
1:A:390:GLY:O	1:A:391:GLN:HB2	2.07	0.53
1:A:905:GLU:HB3	1:A:909:HIS:CE1	2.43	0.53
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.74	0.52
1:A:896:VAL:O	1:A:896:VAL:HG12	2.08	0.52
1:A:462:TYR:CE2	1:A:486:GLN:HG3	2.45	0.52
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.10	0.52
1:A:757:TYR:HA	1:A:758:ASP:CB	2.40	0.52
1:A:744:LYS:O	1:A:748:ASP:OD2	2.29	0.51
1:A:895:THR:O	1:A:896:VAL:HB	2.11	0.51
1:A:842:MET:CE	1:A:871:SER:HB3	2.41	0.51
1:A:568:THR:HG22	1:A:570:GLU:H	1.76	0.50
1:A:899:THR:HG22	1:A:1087:PHE:HD2	1.76	0.50
1:A:759:VAL:CA	1:A:760:SER:CB	2.85	0.50
1:A:574:LEU:HD22	1:A:578:PHE:HD2	1.74	0.50
1:A:475:LEU:HD21	1:A:522:ASN:HB2	1.94	0.50
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.92	0.50
1:A:814:GLU:HG2	1:A:827:THR:OG1	2.12	0.49
1:A:792:LYS:HB3	1:A:818:ALA:HB3	1.93	0.49
1:A:757:TYR:HA	1:A:758:ASP:OD2	2.12	0.49
1:A:622:LEU:HD21	1:A:651:LEU:HD23	1.94	0.49
1:A:746:THR:HG1	1:A:832:PHE:HD2	1.59	0.49
1:A:759:VAL:HG12	1:A:760:SER:O	2.12	0.49
1:A:526:PRO:C	1:A:527:ILE:HD12	2.32	0.49
1:A:558:ILE:O	1:A:591:LYS:HE3	2.13	0.49
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.95	0.49
1:A:526:PRO:O	1:A:527:ILE:HD12	2.13	0.48
1:A:373:LEU:O	1:A:375:ARG:HG3	2.13	0.48
1:A:369:ASP:HA	1:A:406:GLU:O	2.13	0.48
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.49	0.48
1:A:1024:THR:HG23	1:A:1055:LEU:HD13	1.96	0.47
1:A:373:LEU:HD22	1:A:406:GLU:HG3	1.95	0.47
1:A:753:SER:HB3	1:A:809:LYS:HG3	1.95	0.47
1:A:744:LYS:HB3	1:A:744:LYS:HE2	1.70	0.47
1:A:748:ASP:HB2	1:A:770:LYS:NZ	2.30	0.47
1:A:830:ILE:HG21	1:A:878:MET:CE	2.45	0.47
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.45	0.47
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.63	0.47
1:A:657:LEU:HG	1:A:691:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:PHE:HE2	1:A:1048:ILE:HA	1.79	0.46
1:A:579:ARG:CG	1:A:579:ARG:NH1	2.73	0.46
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.98	0.46
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.34	0.46
1:A:1056:THR:HG23	1:A:1059:LYS:HB2	1.98	0.46
1:A:887:THR:HG22	1:A:889:ALA:N	2.31	0.45
1:A:546:GLU:HG3	1:A:547:MET:N	2.30	0.45
1:A:706:SER:O	1:A:710:GLN:HB3	2.16	0.45
1:A:641:ARG:NE	1:A:670:GLU:OE1	2.47	0.45
1:A:964:ASP:C	1:A:966:GLY:H	2.20	0.45
1:A:172:GLU:HB3	1:A:673:HIS:CD2	2.52	0.45
1:A:640:VAL:O	1:A:643:ILE:HG12	2.17	0.45
1:A:682:LEU:O	1:A:682:LEU:HD22	2.17	0.45
1:A:641:ARG:NH1	1:A:670:GLU:OE1	2.48	0.45
1:A:798:ILE:H	1:A:798:ILE:HD12	1.81	0.45
1:A:544:ARG:O	1:A:545:ALA:CB	2.65	0.44
1:A:759:VAL:CA	1:A:760:SER:HB2	2.40	0.44
1:A:373:LEU:N	1:A:374:PRO:CD	2.81	0.44
1:A:748:ASP:HB2	1:A:770:LYS:HZ1	1.83	0.44
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.17	0.44
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	2.00	0.44
1:A:298:LYS:HE3	1:A:861:ASP:OD2	2.18	0.44
1:A:240:THR:HG22	1:A:242:GLY:H	1.83	0.43
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.54	0.43
1:A:375:ARG:NE	1:A:376:ASN:H	2.17	0.43
1:A:756:LYS:HE2	1:A:756:LYS:HB3	1.72	0.43
1:A:744:LYS:O	1:A:748:ASP:CG	2.57	0.43
1:A:842:MET:HE2	1:A:871:SER:HB3	1.99	0.43
1:A:830:ILE:HG21	1:A:878:MET:HE2	1.99	0.43
1:A:1020:LEU:HD22	1:A:1027:LEU:HD11	1.99	0.43
1:A:944:ILE:HD12	1:A:965:PHE:HE1	1.79	0.42
1:A:172:GLU:HB3	1:A:673:HIS:HD2	1.84	0.42
1:A:366:ARG:HH12	1:A:519:LEU:HD22	1.84	0.42
1:A:753:SER:OG	1:A:809:LYS:HG3	2.19	0.42
1:A:500:ASP:O	1:A:503:THR:HG22	2.20	0.42
1:A:777:SER:CB	1:A:778:GLN:CG	2.97	0.42
1:A:935:TYR:O	1:A:939:THR:HB	2.20	0.42
1:A:757:TYR:HA	1:A:758:ASP:CG	2.40	0.42
1:A:806:SER:OG	1:A:808:LYS:HG2	2.20	0.41
1:A:463:TYR:CE2	1:A:501:LYS:HA	2.55	0.41
1:A:730:HIS:O	1:A:734:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:SER:O	1:A:647:LYS:NZ	2.53	0.41
1:A:368:ILE:HG21	1:A:433:ILE:HD11	2.03	0.41
1:A:899:THR:HG22	1:A:1087:PHE:CD2	2.54	0.41
1:A:487:ILE:HD13	1:A:487:ILE:HA	1.90	0.41
1:A:812:TRP:CZ3	2:A:4000:OSD:H15	2.56	0.41
1:A:1048:ILE:O	1:A:1049:GLU:C	2.59	0.41
1:A:289:ASN:HA	1:A:294:ARG:HH21	1.85	0.41
1:A:584:LYS:HA	1:A:616:VAL:HG11	2.04	0.40
1:A:705:GLN:HG3	1:A:839:ARG:CZ	2.51	0.40
1:A:904:ASP:OD1	1:A:904:ASP:N	2.52	0.40
1:A:567:LEU:HD21	1:A:591:LYS:HG2	2.03	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	826/966 (86%)	780 (94%)	40 (5%)	6 (1%)	26 62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	ALA
1	A	758	ASP
1	A	760	SER
1	A	896	VAL
1	A	373	LEU
1	A	527	ILE

### 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	755/864 (87%)	665 (88%)	90 (12%)	6	19

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	165	VAL
1	A	172	GLU
1	A	202	VAL
1	A	219	CYS
1	A	234	LYS
1	A	244	ILE
1	A	245	LEU
1	A	269	ASP
1	A	282	VAL
1	A	285	THR
1	A	298	LYS
1	A	305	VAL
1	A	362	ARG
1	A	373	LEU
1	A	375	ARG
1	A	379	LEU
1	A	381	VAL
1	A	395	CYS
1	A	401	PRO
1	A	406	GLU
1	A	415	GLU
1	A	498	ASN
1	A	520	LEU
1	A	525	HIS
1	A	574	LEU
1	A	575	LEU
1	A	579	ARG
1	A	591	LYS
1	A	603	ILE

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Mol	Chain	Res	Type
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	638	GLU
1	A	647	LYS
1	A	683	LYS
1	A	705	GLN
1	A	717	LEU
1	A	728	MET
1	A	739	ILE
1	A	747	LEU
1	A	749	ILE
1	A	753	SER
1	A	755	GLU
1	A	756	LYS
1	A	758	ASP
1	A	760	SER
1	A	764	ILE
1	A	767	LEU
1	A	775	GLN
1	A	776	ASN
1	A	804	MET
1	A	807	LYS
1	A	808	LYS
1	A	814	GLU
1	A	823	LEU
1	A	825	ASN
1	A	826	GLU
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	865	LEU
1	A	899	THR
1	A	903	LYS
1	A	906	VAL
1	A	907	LEU
1	A	909	HIS
1	A	927	ARG
1	A	939	THR
1	A	949	ASN
1	A	950	ASP
1	A	959	ASN

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Mol	Chain	Res	Type
1	A	967	HIS
1	A	968	ILE
1	A	983	VAL
1	A	988	THR
1	A	1002	THR
1	A	1026	LEU
1	A	1029	ILE
1	A	1032	SER
1	A	1042	LEU
1	A	1043	THR
1	A	1047	ASP
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG
1	A	1056	THR
1	A	1063	ASP
1	A	1078	LYS
1	A	1081	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	HIS
1	A	743	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	0SD	A	4000	-	39,41,41	0.53	1 (2%)	54,60,60	1.43	6 (11%)

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	0SD	A	4000	-	-	0/18/36/36	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	0SD	C16-C21	-2.01	1.37	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	0SD	C12-C13-N1	-4.14	117.35	121.13
2	A	4000	0SD	C13-C14-N6	-2.48	116.14	121.97
2	A	4000	0SD	C16-C15-N3	-2.34	113.25	116.97
2	A	4000	0SD	C16-C15-N2	2.34	120.69	116.97
2	A	4000	0SD	N2-C14-N6	3.53	122.43	116.79
2	A	4000	0SD	C14-C13-N1	6.66	126.82	120.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	0SD	7	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	842/966 (87%)	0.62	79 (9%) 11 5	55, 114, 191, 250	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	8.6
1	A	528	ALA	8.3
1	A	753	SER	6.9
1	A	898	ASN	6.9
1	A	375	ARG	6.8
1	A	376	ASN	6.7
1	A	1091	VAL	5.7
1	A	823	LEU	5.4
1	A	228	THR	5.3
1	A	358	ASP	5.1
1	A	757	TYR	5.1
1	A	373	LEU	4.8
1	A	143	MET	4.8
1	A	545	ALA	4.8
1	A	527	ILE	4.7
1	A	756	LYS	4.5
1	A	751	SER	4.5
1	A	544	ARG	4.5
1	A	211	LEU	4.4
1	A	269	ASP	4.3
1	A	1087	PHE	4.3
1	A	767	LEU	4.3
1	A	322	GLU	4.3
1	A	409	LEU	4.2
1	A	747	LEU	4.2
1	A	1046	GLU	4.1
1	A	834	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	522	ASN	4.1
1	A	377	THR	3.9
1	A	461	LEU	3.9
1	A	268	GLN	3.8
1	A	896	VAL	3.7
1	A	750	LYS	3.6
1	A	287	ILE	3.5
1	A	489	GLY	3.5
1	A	749	ILE	3.5
1	A	218	ASN	3.4
1	A	899	THR	3.4
1	A	272	LEU	3.4
1	A	267	GLU	3.4
1	A	321	GLU	3.3
1	A	1090	LEU	3.2
1	A	219	CYS	3.2
1	A	404	PHE	3.2
1	A	967	HIS	3.2
1	A	1043	THR	3.2
1	A	231	GLN	3.0
1	A	1041	GLN	3.0
1	A	146	GLU	2.9
1	A	1088	LEU	2.9
1	A	968	ILE	2.7
1	A	229	THR	2.7
1	A	220	ILE	2.7
1	A	1045	LYS	2.7
1	A	212	TRP	2.7
1	A	222	ILE	2.6
1	A	778	GLN	2.6
1	A	379	LEU	2.5
1	A	270	PHE	2.5
1	A	821	THR	2.4
1	A	1084	PHE	2.4
1	A	148	GLN	2.4
1	A	147	SER	2.3
1	A	207	LEU	2.3
1	A	905	GLU	2.3
1	A	822	ALA	2.3
1	A	378	ASP	2.3
1	A	1077	ASP	2.3
1	A	462	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	895	THR	2.2
1	A	382	PHE	2.1
1	A	517	SER	2.1
1	A	370	ILE	2.1
1	A	145	GLU	2.0
1	A	519	LEU	2.0
1	A	406	GLU	2.0
1	A	309	THR	2.0
1	A	746	THR	2.0
1	A	1089	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( $\text{\AA}^2$ )	Q<0.9
2	0SD	A	4000	36/36	0.87	0.22	0.21	84,108,132,150	4

## 6.5 Other polymers [i](#)

There are no such residues in this entry.