Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 09:15 AM EST

PDB ID	:	4FAD
Title	:	Design and Synthesis of a Novel Pyrrolidinyl Pyrido Pyrimidinone Derivative as a Potent Inhibitor of PI3Ka and mTOR
Authors	:	Greasley, S.E.; Knighton, D.R.; LaFleur Rogers, C.M.
Deposited on	:	2012-05-22
Resolution	:	2.70 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

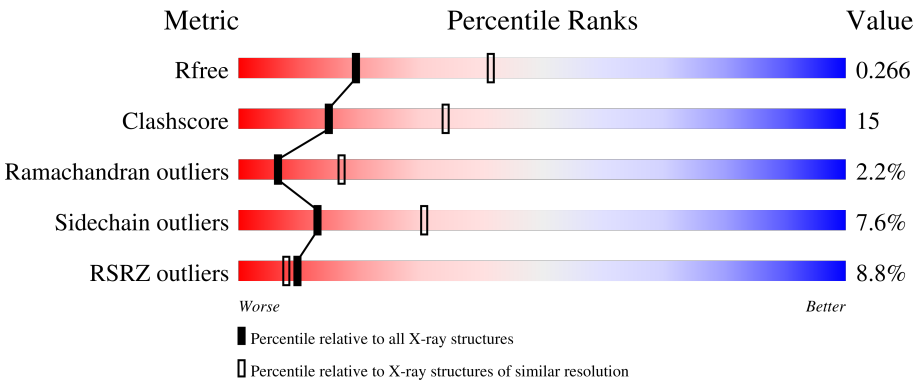
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	8%, 56%, 27%, •, 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6813 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

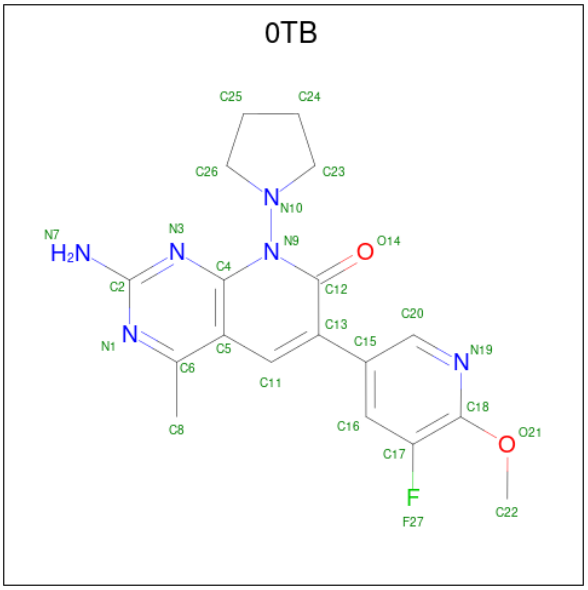
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	839	6781	4363	1150	1233	35	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	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-amino-6-(5-fluoro-6-methoxypyridin-3-yl)-4-methyl-8-(pyrrolidin-1-yl)pyrido [2,3-d]pyrimidin-7(8H)-one (three-letter code: 0TB) (formula: $C_{18}H_{19}FN_6O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	27	18	1	6	2	0	0

- Molecule 3 is water.

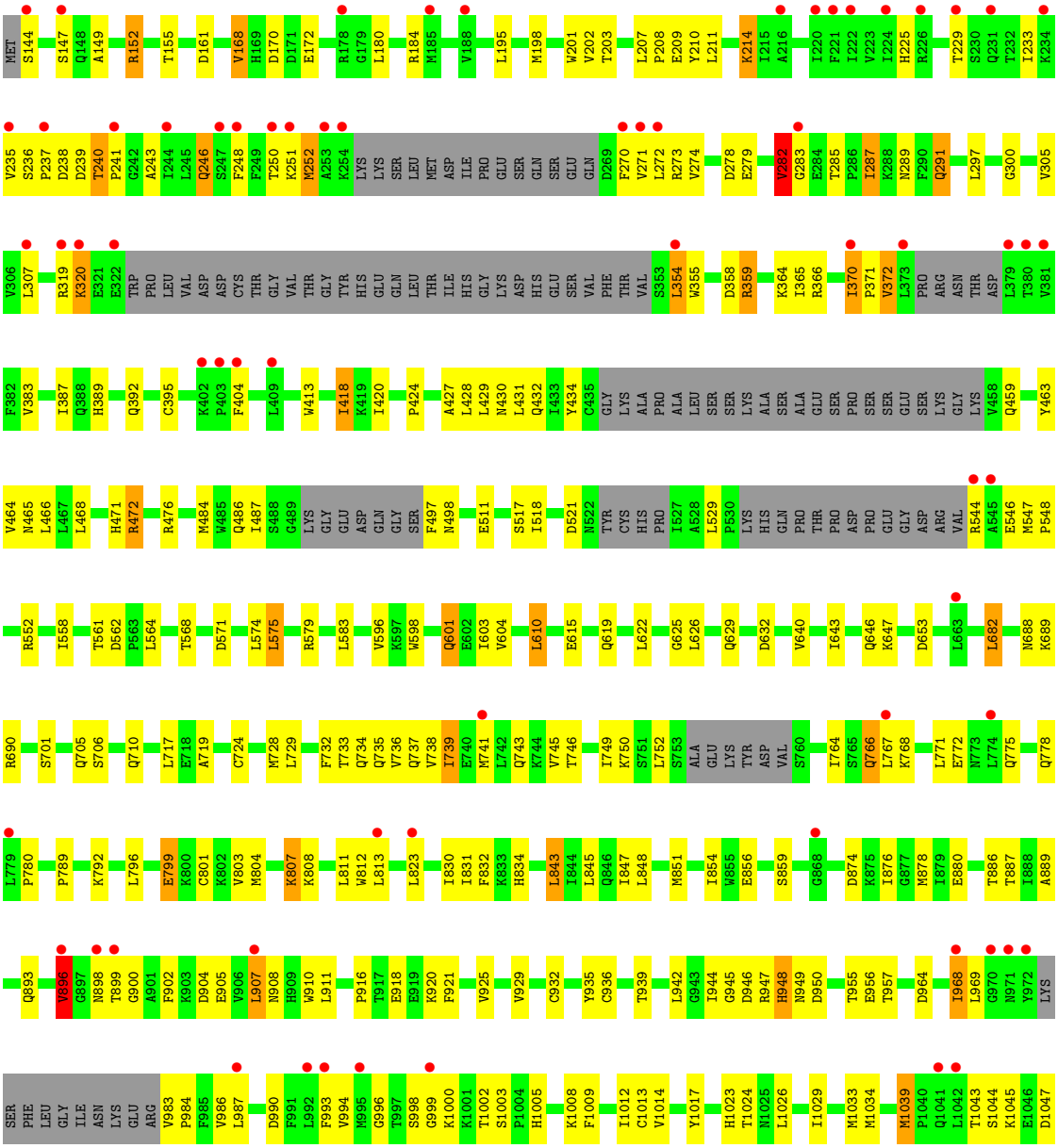
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	5	5	5	0	0

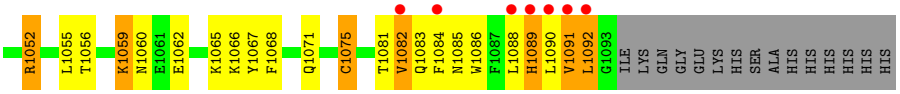
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

Chain A:




R1052
L1055
T1056
K1059
N1060
E1061
E1062
K1065
K1066
Y1067
F1068
Q1071
C1075
T1081
V1082
Q1083
F1084
N1085
W1086
F1087
L1088
H1089
L1090
V1091
L1092
G1093
ILE
LYS
GLN
GLY
GLU
LYS
HIS
SER
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.55Å 67.26Å 107.60Å 90.00° 95.68° 90.00°	Depositor
Resolution (Å)	45.14 – 2.70 45.14 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.14-2.70) 99.2 (45.14-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.69Å)	Xtriage
Refinement program	CNS, BUSTER 2.11.1	Depositor
R, R_{free}	0.262 , 0.265 0.265 , 0.266	Depositor DCC
R_{free} test set	1453 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.49	0/6925	0.75	0/9368

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	6781	0	6820	207	0
2	A	27	0	19	2	0
3	A	5	0	0	0	0
All	All	6813	0	6839	208	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 15.

All (208) 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:1081:THR:O	1:A:1085:ASN:ND2	1.96	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:THR:HG22	1:A:945:GLY:HA2	1.50	0.92
1:A:149:ALA:HA	1:A:152:ARG:NH1	1.85	0.91
1:A:270:PHE:HB3	1:A:307:LEU:HD11	1.57	0.87
1:A:734:GLN:HE21	1:A:780:PRO:HB2	1.43	0.83
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	1.94	0.82
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.62	0.82
1:A:775:GLN:NE2	1:A:796:LEU:H	1.78	0.82
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.66	0.77
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.16	0.76
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.68	0.76
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.51	0.75
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.68	0.74
1:A:983:VAL:CG1	1:A:1082:VAL:HG11	2.17	0.73
1:A:807:LYS:HE3	1:A:807:LYS:H	1.53	0.73
1:A:918:GLU:O	1:A:921:PHE:HB3	1.90	0.71
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.26	0.70
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.22	0.70
1:A:766:GLN:H	1:A:766:GLN:HE21	1.40	0.69
1:A:939:THR:HG22	1:A:945:GLY:CA	2.23	0.68
1:A:775:GLN:HE22	1:A:796:LEU:H	1.39	0.67
1:A:149:ALA:HA	1:A:152:ARG:HH11	1.59	0.67
1:A:983:VAL:HG12	1:A:1082:VAL:HG11	1.77	0.66
1:A:947:ARG:NH1	1:A:948:HIS:CE1	2.64	0.66
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.61	0.66
1:A:907:LEU:HD22	1:A:994:VAL:HG21	1.78	0.65
1:A:235:VAL:HG13	1:A:239:ASP:HB2	1.80	0.64
1:A:944:ILE:HB	1:A:968:ILE:HD12	1.78	0.64
1:A:947:ARG:HD3	1:A:968:ILE:HD13	1.80	0.64
1:A:472:ARG:HG3	1:A:472:ARG:HH11	1.62	0.64
1:A:359:ARG:O	1:A:420:ILE:HG12	1.99	0.63
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.81	0.63
1:A:291:GLN:HE21	1:A:291:GLN:HA	1.63	0.63
1:A:497:PHE:O	1:A:1043:THR:HG21	1.99	0.63
1:A:1089:HIS:ND1	1:A:1089:HIS:C	2.51	0.62
1:A:1091:VAL:HG12	1:A:1091:VAL:O	1.99	0.62
1:A:949:ASN:HB2	1:A:1083:GLN:HE22	1.63	0.62
1:A:766:GLN:H	1:A:766:GLN:NE2	1.99	0.61
1:A:996:GLY:O	1:A:1003:SER:HB2	2.01	0.60
1:A:371:PRO:HG2	1:A:511:GLU:O	2.00	0.60
1:A:239:ASP:O	1:A:287:ILE:HG13	2.02	0.60
1:A:207:LEU:HD21	1:A:211:LEU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:GLN:HG2	1:A:487:ILE:H	1.66	0.60
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.85	0.59
1:A:387:ILE:HD12	1:A:418:ILE:HD13	1.84	0.59
1:A:270:PHE:HB3	1:A:307:LEU:CD1	2.32	0.59
1:A:916:PRO:HD2	1:A:920:LYS:HD2	1.85	0.59
1:A:184:ARG:HH11	1:A:719:ALA:HA	1.68	0.59
1:A:558:ILE:O	1:A:561:THR:HG22	2.03	0.59
1:A:1081:THR:C	1:A:1085:ASN:HD22	1.99	0.59
1:A:271:VAL:HG21	1:A:282:VAL:HG13	1.86	0.58
1:A:1008:LYS:HG2	1:A:1012:ILE:HD11	1.84	0.58
1:A:241:PRO:HD3	1:A:285:THR:O	2.04	0.58
1:A:251:LYS:O	1:A:251:LYS:HD3	2.03	0.58
1:A:149:ALA:HA	1:A:152:ARG:HH12	1.65	0.58
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.85	0.58
1:A:764:ILE:O	1:A:768:LYS:HG2	2.04	0.57
1:A:568:THR:HG23	1:A:571:ASP:H	1.69	0.57
1:A:370:ILE:HD12	1:A:372:VAL:O	2.05	0.56
1:A:925:VAL:O	1:A:929:VAL:HG23	2.05	0.56
1:A:214:LYS:HD3	1:A:297:LEU:O	2.05	0.56
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.71	0.56
1:A:1091:VAL:O	1:A:1092:LEU:HG	2.06	0.56
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.87	0.56
1:A:734:GLN:O	1:A:738:VAL:HG23	2.06	0.56
1:A:921:PHE:O	1:A:925:VAL:HG23	2.06	0.56
1:A:170:ASP:OD1	1:A:172:GLU:HB2	2.06	0.55
1:A:739:ILE:O	1:A:743:GLN:HG3	2.06	0.55
1:A:640:VAL:O	1:A:643:ILE:HG12	2.06	0.55
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.71	0.55
1:A:1081:THR:C	1:A:1085:ASN:ND2	2.59	0.55
1:A:1009:PHE:HA	1:A:1012:ILE:HD12	1.88	0.55
1:A:547:MET:HE1	1:A:552:ARG:HA	1.89	0.55
1:A:273:ARG:HG3	1:A:274:VAL:N	2.21	0.54
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.37	0.54
1:A:801:CYS:HA	1:A:812:TRP:O	2.08	0.54
1:A:955:THR:C	1:A:957:THR:H	2.11	0.54
1:A:983:VAL:HG11	1:A:1082:VAL:HG11	1.89	0.54
1:A:998:SER:O	1:A:1000:LYS:N	2.41	0.54
1:A:896:VAL:HG21	1:A:899:THR:HB	1.91	0.53
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.44	0.53
1:A:1060:ASN:OD1	1:A:1062:GLU:HB2	2.08	0.53
1:A:418:ILE:HD12	1:A:418:ILE:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:HIS:HD2	1:A:1086:TRP:CZ3	2.27	0.53
1:A:246:GLN:O	1:A:250:THR:HB	2.08	0.53
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.20	0.53
1:A:767:LEU:HG	1:A:803:VAL:HG23	1.89	0.53
1:A:896:VAL:CG2	1:A:899:THR:HB	2.39	0.53
1:A:830:ILE:CG2	1:A:878:MET:HB2	2.39	0.53
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.90	0.52
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.44	0.52
1:A:184:ARG:NH1	1:A:719:ALA:HA	2.24	0.52
1:A:248:PHE:O	1:A:252:MET:HG3	2.10	0.52
1:A:615:GLU:O	1:A:619:GLN:HB2	2.09	0.52
1:A:625:GLY:O	1:A:629:GLN:HG3	2.10	0.52
1:A:1002:THR:HG22	1:A:1003:SER:H	1.75	0.52
1:A:653:ASP:OD2	1:A:688:ASN:ND2	2.42	0.52
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.90	0.51
1:A:689:LYS:HG2	1:A:728:MET:SD	2.49	0.51
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.92	0.51
1:A:887:THR:HG23	1:A:950:ASP:O	2.11	0.51
1:A:947:ARG:NH1	1:A:948:HIS:HE1	2.08	0.51
1:A:596:VAL:HG13	1:A:603:ILE:HG22	1.94	0.50
1:A:735:GLN:O	1:A:739:ILE:HG23	2.12	0.50
1:A:1056:THR:OG1	1:A:1059:LYS:HG3	2.12	0.49
1:A:472:ARG:HG3	1:A:472:ARG:NH1	2.27	0.49
1:A:272:LEU:HB3	1:A:305:VAL:CG1	2.42	0.49
1:A:887:THR:HG22	1:A:889:ALA:H	1.77	0.49
1:A:144:SER:HB3	1:A:147:SER:HB3	1.94	0.49
1:A:180:LEU:HD22	1:A:682:LEU:HD12	1.94	0.49
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.12	0.49
1:A:240:THR:HG23	1:A:243:ALA:HB3	1.94	0.48
1:A:354:LEU:HD22	1:A:529:LEU:HB2	1.94	0.48
1:A:274:VAL:HG23	1:A:279:GLU:O	2.14	0.48
1:A:632:ASP:HB3	1:A:1033:MET:HE3	1.95	0.48
1:A:746:THR:O	1:A:750:LYS:HB2	2.12	0.48
1:A:893:GLN:HA	1:A:896:VAL:O	2.14	0.48
1:A:880:GLU:O	2:A:1201:0TB:H2	2.13	0.48
1:A:287:ILE:N	1:A:287:ILE:HD12	2.29	0.48
1:A:320:LYS:HD2	1:A:320:LYS:H	1.79	0.47
1:A:969:LEU:HD13	1:A:1039:MET:CE	2.44	0.47
1:A:1052:ARG:HG2	1:A:1052:ARG:HH11	1.79	0.47
1:A:389:HIS:O	1:A:392:GLN:HB3	2.15	0.47
1:A:365:ILE:HD12	1:A:383:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:SER:O	1:A:710:GLN:HB3	2.15	0.47
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.97	0.47
1:A:987:LEU:HB3	1:A:1075:CYS:SG	2.54	0.47
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.97	0.47
1:A:767:LEU:O	1:A:771:LEU:HG	2.15	0.47
1:A:291:GLN:HA	1:A:291:GLN:NE2	2.30	0.46
1:A:804:MET:HE3	1:A:831:ILE:HG23	1.97	0.46
1:A:1005:HIS:CE1	1:A:1008:LYS:HZ1	2.33	0.46
1:A:240:THR:HG23	1:A:243:ALA:CB	2.46	0.46
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.98	0.46
1:A:1017:TYR:OH	1:A:1056:THR:HG22	2.16	0.46
1:A:929:VAL:HG13	1:A:1009:PHE:HB2	1.98	0.46
1:A:236:SER:O	1:A:287:ILE:HD11	2.16	0.46
1:A:768:LYS:HE2	1:A:801:CYS:O	2.16	0.46
1:A:764:ILE:HG23	1:A:768:LYS:HE3	1.98	0.45
1:A:1024:THR:HA	1:A:1055:LEU:HD13	1.98	0.45
1:A:807:LYS:HE3	1:A:807:LYS:N	2.26	0.45
1:A:908:ASN:ND2	1:A:994:VAL:HA	2.30	0.45
1:A:271:VAL:CG2	1:A:282:VAL:HG13	2.46	0.45
1:A:690:ARG:NH1	1:A:789:PRO:HG2	2.31	0.45
1:A:799:GLU:H	1:A:799:GLU:HG3	1.61	0.45
1:A:811:LEU:HD23	1:A:813:LEU:HD21	1.98	0.45
1:A:168:VAL:HG13	1:A:170:ASP:H	1.81	0.45
1:A:947:ARG:NH2	1:A:964:ASP:O	2.50	0.45
1:A:364:LYS:HD2	1:A:413:TRP:CE2	2.52	0.45
1:A:932:CYS:O	1:A:936:CYS:SG	2.70	0.45
1:A:198:MET:CB	1:A:282:VAL:HG21	2.48	0.44
1:A:732:PHE:O	1:A:736:VAL:HG23	2.18	0.44
1:A:203:THR:O	1:A:289:ASN:HB3	2.17	0.44
1:A:152:ARG:HH11	1:A:152:ARG:HB2	1.83	0.44
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.32	0.44
1:A:431:LEU:O	1:A:463:TYR:HA	2.18	0.43
1:A:464:VAL:HB	1:A:484:MET:HG2	2.00	0.43
1:A:622:LEU:HD13	1:A:647:LYS:O	2.18	0.43
1:A:210:TYR:OH	1:A:856:GLU:HG3	2.18	0.43
1:A:896:VAL:HG13	1:A:900:GLY:H	1.82	0.43
1:A:944:ILE:HB	1:A:968:ILE:CD1	2.45	0.43
1:A:1029:ILE:O	1:A:1033:MET:HB2	2.17	0.43
1:A:278:ASP:OD2	1:A:792:LYS:NZ	2.52	0.43
1:A:601:GLN:HE21	1:A:601:GLN:HB2	1.45	0.43
1:A:598:TRP:CE3	1:A:604:VAL:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:GLN:HG2	1:A:487:ILE:N	2.31	0.43
1:A:847:ILE:HG21	1:A:942:LEU:HD21	2.00	0.43
1:A:874:ASP:O	1:A:876:ILE:HG22	2.19	0.43
1:A:935:TYR:O	1:A:939:THR:CB	2.67	0.43
1:A:246:GLN:HE21	1:A:246:GLN:HA	1.84	0.43
2:A:1201:0TB:H14	2:A:1201:0TB:H1	1.81	0.42
1:A:579:ARG:HB2	1:A:610:LEU:HD11	2.01	0.42
1:A:848:LEU:HD12	1:A:851:MET:CE	2.49	0.42
1:A:201:TRP:CE3	1:A:291:GLN:HB2	2.54	0.42
1:A:207:LEU:HD21	1:A:211:LEU:CB	2.50	0.42
1:A:424:PRO:HD2	1:A:427:ALA:HB2	2.02	0.42
1:A:945:GLY:O	1:A:986:VAL:HG23	2.20	0.42
1:A:355:TRP:NE1	1:A:601:GLN:NE2	2.67	0.42
1:A:745:VAL:O	1:A:749:ILE:HD13	2.20	0.42
1:A:207:LEU:HD23	1:A:208:PRO:O	2.20	0.42
1:A:466:LEU:HD11	1:A:476:ARG:HH11	1.84	0.42
1:A:562:ASP:OD2	1:A:1052:ARG:NH1	2.53	0.42
1:A:1083:GLN:NE2	1:A:1083:GLN:HA	2.35	0.42
1:A:366:ARG:HB2	1:A:517:SER:HB2	2.01	0.41
1:A:910:TRP:HE3	1:A:911:LEU:HD23	1.85	0.41
1:A:236:SER:O	1:A:238:ASP:N	2.53	0.41
1:A:701:SER:O	1:A:705:GLN:HG2	2.21	0.41
1:A:767:LEU:HD21	1:A:811:LEU:HG	2.01	0.41
1:A:147:SER:HB2	1:A:319:ARG:NH2	2.34	0.41
1:A:273:ARG:HG3	1:A:274:VAL:H	1.83	0.41
1:A:1043:THR:O	1:A:1047:ASP:HB2	2.20	0.41
1:A:546:GLU:HG3	1:A:547:MET:H	1.85	0.41
1:A:990:ASP:O	1:A:994:VAL:HG23	2.21	0.41
1:A:207:LEU:CD2	1:A:211:LEU:HB2	2.49	0.41
1:A:935:TYR:O	1:A:939:THR:HB	2.21	0.41
1:A:568:THR:HG22	1:A:571:ASP:CG	2.41	0.41
1:A:741:MET:O	1:A:745:VAL:HG23	2.21	0.41
1:A:434:TYR:HA	1:A:459:GLN:O	2.20	0.40
1:A:155:THR:HG23	1:A:161:ASP:HA	2.03	0.40
1:A:320:LYS:H	1:A:320:LYS:CD	2.34	0.40
1:A:768:LYS:O	1:A:772:GLU:HG2	2.21	0.40
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.56	0.40
1:A:152:ARG:NH1	1:A:152:ARG:HB2	2.36	0.40
1:A:430:ASN:OD1	1:A:432:GLN:NE2	2.52	0.40
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.46	0.40
1:A:184:ARG:HD3	1:A:719:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:PHE:CZ	1:A:1088:LEU:HD21	2.56	0.40
1:A:466:LEU:HD11	1:A:476:ARG:HD3	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	819/966 (85%)	713 (87%)	88 (11%)	18 (2%)	6 17

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	ASP
1	A	548	PRO
1	A	984	PRO
1	A	999	GLY
1	A	1045	LYS
1	A	1092	LEU
1	A	237	PRO
1	A	282	VAL
1	A	896	VAL
1	A	902	PHE
1	A	968	ILE
1	A	1044	SER
1	A	904	ASP
1	A	956	GLU
1	A	752	LEU
1	A	283	GLY
1	A	1091	VAL
1	A	372	VAL

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	750/864 (87%)	693 (92%)	57 (8%)	13 30

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	168	VAL
1	A	195	LEU
1	A	214	LYS
1	A	225	HIS
1	A	229	THR
1	A	240	THR
1	A	246	GLN
1	A	252	MET
1	A	282	VAL
1	A	287	ILE
1	A	291	GLN
1	A	320	LYS
1	A	354	LEU
1	A	358	ASP
1	A	359	ARG
1	A	370	ILE
1	A	404	PHE
1	A	418	ILE
1	A	472	ARG
1	A	498	ASN
1	A	518	ILE
1	A	544	ARG
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	626	LEU
1	A	646	GLN
1	A	682	LEU

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Mol	Chain	Res	Type
1	A	717	LEU
1	A	729	LEU
1	A	739	ILE
1	A	766	GLN
1	A	778	GLN
1	A	799	GLU
1	A	807	LYS
1	A	808	LYS
1	A	823	LEU
1	A	832	PHE
1	A	843	LEU
1	A	845	LEU
1	A	886	THR
1	A	896	VAL
1	A	898	ASN
1	A	907	LEU
1	A	946	ASP
1	A	948	HIS
1	A	1026	LEU
1	A	1039	MET
1	A	1052	ARG
1	A	1059	LYS
1	A	1066	LYS
1	A	1075	CYS
1	A	1082	VAL
1	A	1089	HIS
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	246	GLN
1	A	291	GLN
1	A	304	HIS
1	A	391	GLN
1	A	392	GLN
1	A	483	HIS
1	A	549	ASN
1	A	554	GLN
1	A	565	ASN
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	601	GLN
1	A	634	ASN
1	A	734	GLN
1	A	737	GLN
1	A	743	GLN
1	A	762	GLN
1	A	766	GLN
1	A	773	ASN
1	A	775	GLN
1	A	778	GLN
1	A	834	HIS
1	A	893	GLN
1	A	908	ASN
1	A	948	HIS
1	A	959	ASN
1	A	1023	HIS
1	A	1083	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	0TB	A	1201	-	26,30,30	1.31	4 (15%)	33,44,44	2.24	5 (15%)

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	0TB	A	1201	-	-	2/6/17/17	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	0TB	C2-N7	3.12	1.40	1.33
2	A	1201	0TB	C13-C12	2.90	1.50	1.46
2	A	1201	0TB	O21-C18	2.69	1.39	1.35
2	A	1201	0TB	C5-C4	-2.68	1.38	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	0TB	C22-O21-C18	-9.12	108.17	117.21
2	A	1201	0TB	O14-C12-C13	-5.84	117.83	125.72
2	A	1201	0TB	O21-C18-N19	3.21	124.08	120.35
2	A	1201	0TB	C16-C17-C18	-2.20	119.50	121.83
2	A	1201	0TB	C4-C5-C11	2.06	121.18	118.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	0TB	N19-C18-O21-C22
2	A	1201	0TB	C17-C18-O21-C22

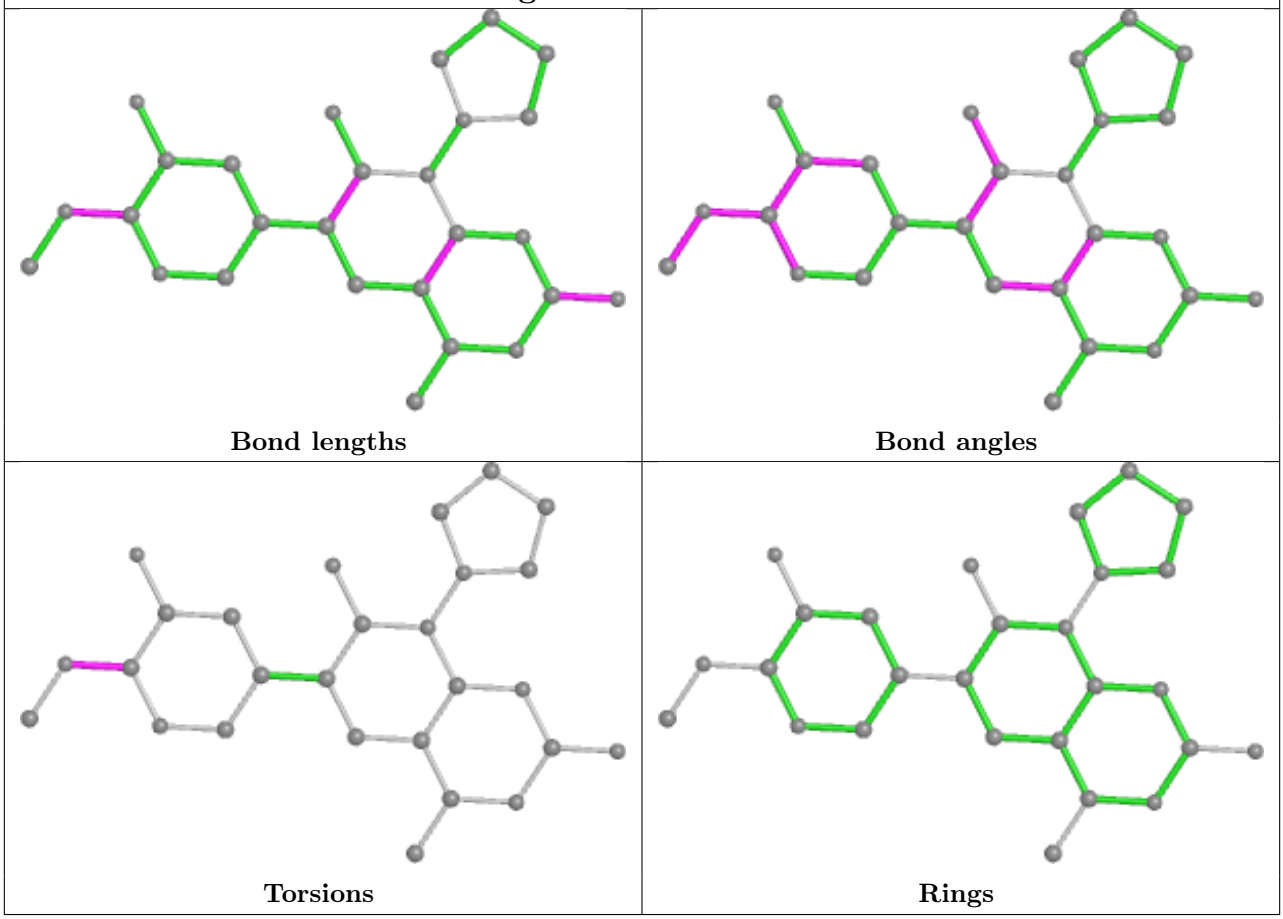
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	0TB	2	0

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

Ligand 0TB A 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	839/966 (86%)	0.70	74 (8%) 10 8	41, 79, 118, 149	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	898	ASN	7.9
1	A	899	THR	7.2
1	A	774	LEU	6.5
1	A	995	MET	6.3
1	A	379	LEU	5.3
1	A	1042	LEU	4.8
1	A	254	LYS	4.7
1	A	237	PRO	4.7
1	A	767	LEU	4.3
1	A	1092	LEU	4.2
1	A	779	LEU	4.1
1	A	270	PHE	4.1
1	A	322	GLU	4.0
1	A	147	SER	4.0
1	A	1041	GLN	4.0
1	A	972	TYR	3.9
1	A	999	GLY	3.9
1	A	1082	VAL	3.9
1	A	235	VAL	3.8
1	A	220	ILE	3.7
1	A	231	GLN	3.7
1	A	226	ARG	3.6
1	A	823	LEU	3.6
1	A	970	GLY	3.6
1	A	251	LYS	3.6
1	A	987	LEU	3.5
1	A	907	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	3.3
1	A	354	LEU	3.3
1	A	404	PHE	3.3
1	A	241	PRO	3.3
1	A	896	VAL	3.3
1	A	370	ILE	3.3
1	A	320	LYS	3.2
1	A	234	LYS	3.2
1	A	307	LEU	3.1
1	A	993	PHE	3.1
1	A	1084	PHE	3.1
1	A	409	LEU	2.9
1	A	250	THR	2.9
1	A	248	PHE	2.9
1	A	1090	LEU	2.9
1	A	271	VAL	2.9
1	A	1088	LEU	2.8
1	A	545	ALA	2.8
1	A	283	GLY	2.8
1	A	253	ALA	2.7
1	A	222	ILE	2.7
1	A	1091	VAL	2.7
1	A	971	ASN	2.7
1	A	373	LEU	2.7
1	A	272	LEU	2.7
1	A	188	VAL	2.6
1	A	992	LEU	2.6
1	A	319	ARG	2.4
1	A	403	PRO	2.4
1	A	968	ILE	2.3
1	A	813	LEU	2.3
1	A	380	THR	2.3
1	A	224	ILE	2.3
1	A	178	ARG	2.3
1	A	402	LYS	2.3
1	A	663	LEU	2.2
1	A	244	ILE	2.2
1	A	247	SER	2.2
1	A	221	PHE	2.2
1	A	741	MET	2.2
1	A	185	MET	2.2
1	A	544	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1089	HIS	2.1
1	A	381	VAL	2.1
1	A	868	GLY	2.1
1	A	144	SER	2.1
1	A	229	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

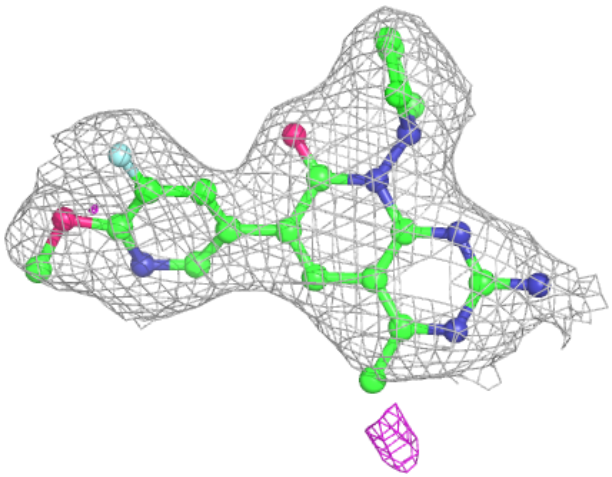
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

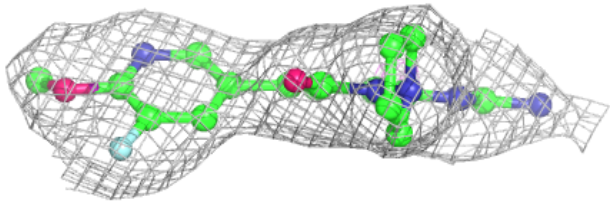
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	0TB	A	1201	27/27	0.95	0.15	52,54,55,55	0

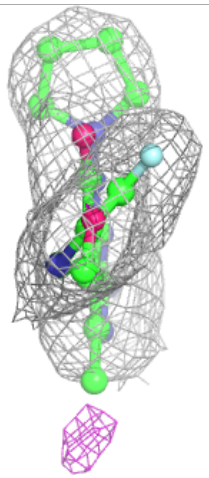
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 0TB A 1201:

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







6.5 Other polymers (i)

There are no such residues in this entry.