Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 05:37 PM EST

PDB ID	:	3T8M
Title	:	Rational Design of PI3K-alpha Inhibitors that Exhibit Selectivity Over the PI3K-beta Isoform
Authors	:	Murray, J.M.; Wiesmann, C.
Deposited on	:	2011-08-01
Resolution	:	2.50 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 ⓘ 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 ⓘ) were used in the production of this report:

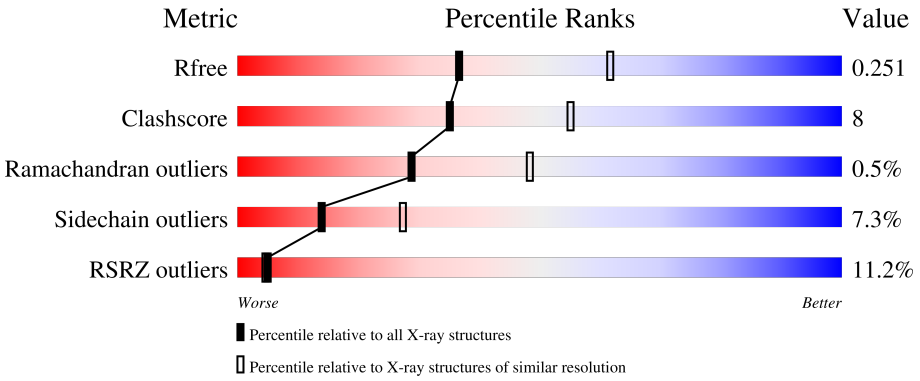
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	10% 65% 20% · 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6865 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.

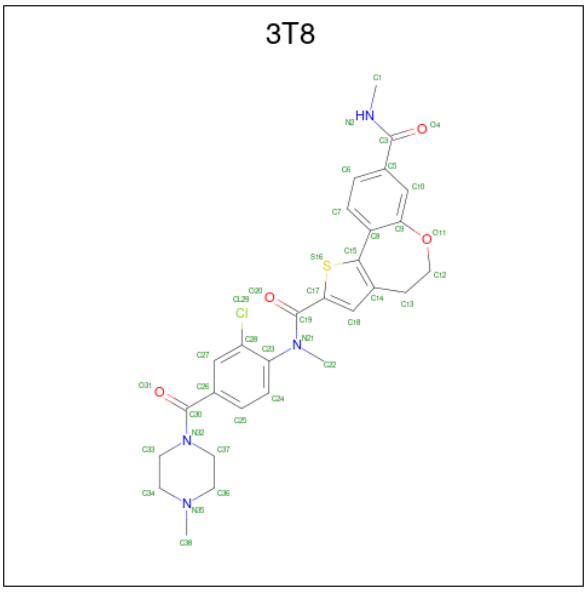
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	841	6812	4371	1164	1242	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 N 2 -{2-chloro-4-[(4-methylpiperazin-1-yl)carbonyl]phenyl}-N 2 ,N 8 -dimethyl-4,5-dihydrothieno[3,2-d][1]benzoxepine-2,8-dicarboxamide (three-letter code: 3T8) (formula: $C_{28}H_{29}ClN_4O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			38	28	1	4	4	1		

- Molecule 3 is water.

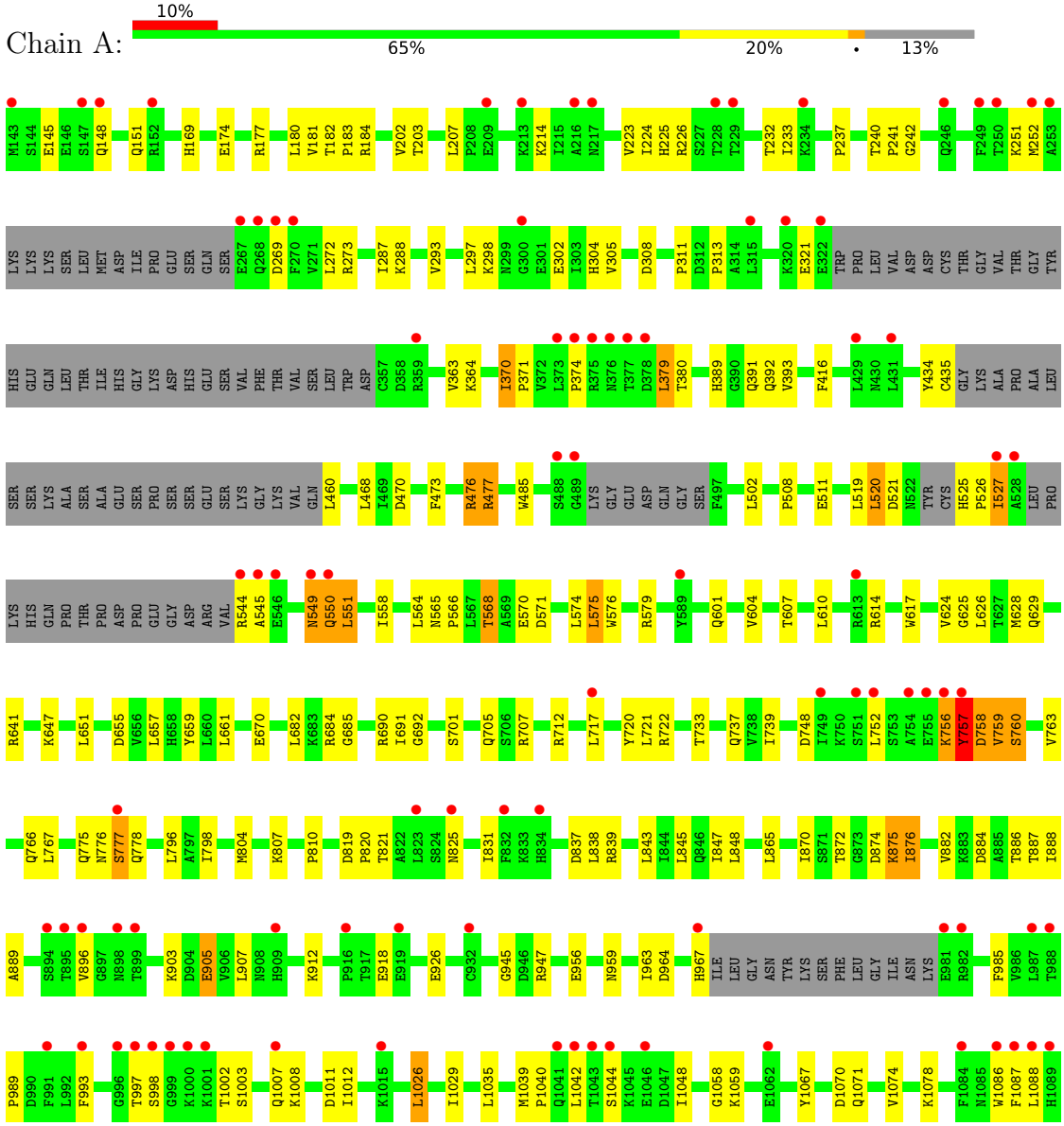
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		

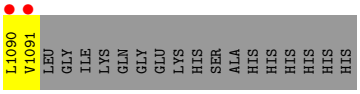
3 Residue-property plots (i)

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:




L1090
V1091
LEU
GLY
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	143.22Å 67.65Å 106.63Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	19.86 – 2.50 19.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.86-2.50) 99.8 (19.86-2.50)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.50Å)	Xtriage
Refinement program	PHENIX dev_833	Depositor
R, R_{free}	0.204 , 0.254 0.201 , 0.251	Depositor DCC
R_{free} test set	1744 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.1	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	0.96	EDS
Total number of atoms	6865	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3T8

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	0.62	0/6958	0.84	11/9412 (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	5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	712	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	A	684	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	777	SER	N-CA-C	-6.87	92.46	111.00
1	A	684	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	870	ILE	CG1-CB-CG2	-6.27	97.61	111.40
1	A	551	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	A	659	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	470	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	847	ILE	CG1-CB-CG2	-5.30	99.73	111.40
1	A	1026	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	661	LEU	CB-CG-CD2	-5.02	102.47	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	LYS	Peptide
1	A	757	TYR	Peptide
1	A	759	VAL	Peptide
1	A	776	ASN	Peptide
1	A	777	SER	Peptide

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	6812	0	6843	112	0
2	A	38	0	29	3	0
3	A	15	0	0	1	0
All	All	6865	0	6872	112	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 8.

All (112) 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:705:GLN:NE2	1:A:837:ASP:OD1	1.90	1.03
1:A:804:MET:HE2	1:A:831:ILE:HG12	1.67	0.76
1:A:759:VAL:HA	1:A:760:SER:HB2	1.70	0.74
1:A:947:ARG:NH2	1:A:963:ILE:O	2.23	0.71
1:A:549:ASN:OD1	1:A:550:GLN:NE2	2.24	0.70
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.24	0.70
1:A:819:ASP:OD1	1:A:821:THR:OG1	2.13	0.67
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.77	0.67
1:A:223:VAL:HG22	1:A:232:THR:HG23	1.76	0.66
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.78	0.66
1:A:887:THR:HG22	1:A:889:ALA:H	1.62	0.64
1:A:174:GLU:OE2	1:A:177:ARG:NH1	2.30	0.64
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.81	0.63
1:A:182:THR:HB	1:A:183:PRO:HD3	1.82	0.61
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.83	0.61
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.39	0.58
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.85	0.58
1:A:756:LYS:HA	1:A:757:TYR:O	2.04	0.57
1:A:756:LYS:HD2	1:A:807:LYS:HA	1.86	0.57
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.87	0.57
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.05	0.57
1:A:181:VAL:HG22	1:A:184:ARG:HH22	1.70	0.56
1:A:273:ARG:NH2	1:A:821:THR:OG1	2.38	0.56
1:A:1086:TRP:HE3	1:A:1087:PHE:H	1.54	0.55
1:A:224:ILE:HD12	1:A:233:ILE:HD13	1.89	0.55
1:A:181:VAL:HG22	1:A:184:ARG:NH2	2.22	0.54
1:A:912:LYS:NZ	1:A:918:GLU:OE2	2.39	0.54
1:A:473:PHE:HD2	1:A:527:ILE:HD13	1.73	0.54
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.91	0.53
1:A:778:GLN:N	1:A:778:GLN:OE1	2.42	0.53
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.73	0.52
1:A:804:MET:HE3	1:A:810:PRO:HG2	1.90	0.52
1:A:1086:TRP:HZ3	1:A:1090:LEU:HD21	1.74	0.52
1:A:476:ARG:HB3	1:A:520:LEU:HD23	1.92	0.52
1:A:775:GLN:HE22	1:A:796:LEU:N	2.07	0.52
1:A:874:ASP:OD1	1:A:875:LYS:NZ	2.40	0.51
1:A:1002:THR:HG22	1:A:1003:SER:H	1.75	0.51
1:A:733:THR:O	1:A:737:GLN:HG3	2.12	0.50
1:A:705:GLN:HG3	1:A:839:ARG:CZ	2.41	0.50
1:A:379:LEU:HD13	1:A:380:THR:H	1.78	0.49
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.95	0.48
1:A:180:LEU:C	1:A:183:PRO:HD2	2.33	0.48
1:A:875:LYS:HD3	1:A:875:LYS:HA	1.63	0.48
1:A:739:ILE:HD13	1:A:872:THR:HB	1.93	0.48
1:A:1086:TRP:CZ3	1:A:1090:LEU:HD21	2.48	0.48
1:A:625:GLY:O	1:A:629:GLN:HG3	2.14	0.48
1:A:311:PRO:O	1:A:313:PRO:HD3	2.13	0.48
1:A:657:LEU:HD11	1:A:690:ARG:HD3	1.96	0.48
1:A:604:VAL:O	1:A:607:THR:HB	2.13	0.47
1:A:759:VAL:HG13	1:A:763:VAL:HB	1.95	0.47
1:A:964:ASP:CG	2:A:1:3T8:H22B	2.35	0.47
1:A:145:GLU:HA	1:A:148:GLN:OE1	2.15	0.47
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.96	0.47
1:A:945:GLY:O	1:A:985:PHE:HA	2.15	0.47
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.14	0.47
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:VAL:CA	1:A:760:SER:HB2	2.43	0.47
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.47	0.46
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.79	0.46
1:A:798:ILE:HD12	1:A:798:ILE:H	1.81	0.46
1:A:308:ASP:N	1:A:308:ASP:OD1	2.46	0.46
1:A:251:LYS:O	1:A:251:LYS:HD3	2.16	0.46
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.97	0.46
1:A:1058:GLY:C	1:A:1059:LYS:HD3	2.37	0.45
1:A:389:HIS:O	1:A:392:GLN:HB3	2.16	0.45
1:A:565:ASN:OD1	1:A:566:PRO:HD2	2.17	0.45
1:A:748:ASP:O	1:A:752:LEU:HG	2.17	0.45
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.16	0.45
1:A:287:ILE:HD12	1:A:288:LYS:N	2.32	0.45
1:A:964:ASP:CB	2:A:1:3T8:H22B	2.47	0.45
1:A:202:VAL:CG1	1:A:203:THR:N	2.80	0.44
1:A:1086:TRP:C	1:A:1088:LEU:H	2.20	0.44
1:A:391:GLN:HG3	1:A:502:LEU:HD21	1.99	0.44
1:A:169:HIS:HE1	3:A:8:HOH:O	1.99	0.44
1:A:721:LEU:HA	1:A:721:LEU:HD23	1.78	0.44
1:A:202:VAL:HG12	1:A:203:THR:N	2.33	0.44
1:A:477:ARG:HA	1:A:520:LEU:HB3	2.00	0.44
1:A:551:LEU:HA	1:A:551:LEU:HD23	1.75	0.44
1:A:701:SER:O	1:A:705:GLN:HG2	2.17	0.44
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.18	0.44
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.53	0.43
1:A:240:THR:HG22	1:A:242:GLY:H	1.82	0.43
1:A:882:VAL:HG23	2:A:1:3T8:H12	2.00	0.43
1:A:1029:ILE:HD12	1:A:1029:ILE:HA	1.86	0.43
1:A:884:ASP:O	1:A:956:GLU:HG3	2.18	0.43
1:A:874:ASP:O	1:A:876:ILE:HG22	2.19	0.43
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.47	0.43
1:A:370:ILE:HG12	1:A:371:PRO:HD2	2.01	0.43
1:A:624:VAL:O	1:A:628:MET:HG2	2.19	0.42
1:A:886:THR:HG22	1:A:887:THR:H	1.84	0.42
1:A:641:ARG:HE	1:A:670:GLU:CD	2.22	0.42
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.86	0.42
1:A:886:THR:HG22	1:A:887:THR:N	2.34	0.42
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.54	0.42
1:A:180:LEU:O	1:A:183:PRO:HD2	2.20	0.42
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.49	0.42
1:A:240:THR:HG23	1:A:241:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HD12	1:A:233:ILE:H	1.84	0.42
1:A:371:PRO:HG2	1:A:511:GLU:O	2.20	0.42
1:A:757:TYR:CD2	1:A:757:TYR:N	2.87	0.41
1:A:370:ILE:HG12	1:A:371:PRO:CD	2.50	0.41
1:A:819:ASP:HA	1:A:820:PRO:HD2	1.88	0.41
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.21	0.41
1:A:997:THR:HG22	1:A:998:SER:N	2.35	0.41
1:A:905:GLU:HB3	1:A:993:PHE:CZ	2.56	0.41
1:A:485:TRP:CH2	1:A:508:PRO:HD3	2.56	0.41
1:A:293:VAL:O	1:A:297:LEU:HG	2.20	0.41
1:A:568:THR:HG1	1:A:571:ASP:CG	2.23	0.41
1:A:214:LYS:NZ	1:A:297:LEU:HA	2.35	0.40
1:A:379:LEU:HD13	1:A:380:THR:HG22	2.03	0.40
1:A:364:LYS:HB3	1:A:519:LEU:HB3	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	825/966 (85%)	780 (94%)	41 (5%)	4 (0%)	29 48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	ASP
1	A	896	VAL
1	A	545	ALA
1	A	527	ILE

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	754/864 (87%)	699 (93%)	55 (7%)	14 27

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	LEU
1	A	226	ARG
1	A	252	MET
1	A	269	ASP
1	A	298	LYS
1	A	370	ILE
1	A	374	PRO
1	A	379	LEU
1	A	393	VAL
1	A	435	CYS
1	A	476	ARG
1	A	477	ARG
1	A	520	LEU
1	A	521	ASP
1	A	544	ARG
1	A	549	ASN
1	A	550	GLN
1	A	568	THR
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	682	LEU
1	A	707	ARG
1	A	717	LEU
1	A	757	TYR
1	A	758	ASP

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Mol	Chain	Res	Type
1	A	760	SER
1	A	766	GLN
1	A	767	LEU
1	A	825	ASN
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	875	LYS
1	A	876	ILE
1	A	888	ILE
1	A	903	LYS
1	A	905	GLU
1	A	907	LEU
1	A	926	GLU
1	A	959	ASN
1	A	967	HIS
1	A	989	PRO
1	A	1011	ASP
1	A	1026	LEU
1	A	1042	LEU
1	A	1044	SER
1	A	1078	LYS
1	A	1091	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	304	HIS
1	A	549	ASN
1	A	550	GLN
1	A	766	GLN
1	A	775	GLN
1	A	1007	GLN

5.3.3 RNA

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	3T8	A	1	-	36,42,42	0.97	1 (2%)	50,61,61	1.70	11 (22%)

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	3T8	A	1	-	-	0/22/46/46	0/4/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	3T8	C3-N2	2.92	1.37	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	3T8	C24-C23-N21	4.29	124.26	118.74
2	A	1	3T8	C1-N2-C3	4.14	126.57	121.89
2	A	1	3T8	C17-C19-N21	3.42	126.65	118.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	3T8	O20-C19-N21	-3.34	116.38	121.47
2	A	1	3T8	C15-C8-C9	3.25	124.40	119.69
2	A	1	3T8	C27-C28-C23	3.24	123.37	120.74
2	A	1	3T8	O11-C9-C10	3.10	121.43	116.95
2	A	1	3T8	O31-C30-N32	-2.84	117.64	122.34
2	A	1	3T8	C26-C30-N32	2.58	122.00	118.72
2	A	1	3T8	C14-C15-S16	-2.22	107.50	111.79
2	A	1	3T8	C33-C34-N35	-2.16	108.36	110.80

There are no chirality outliers.

There are no torsion outliers.

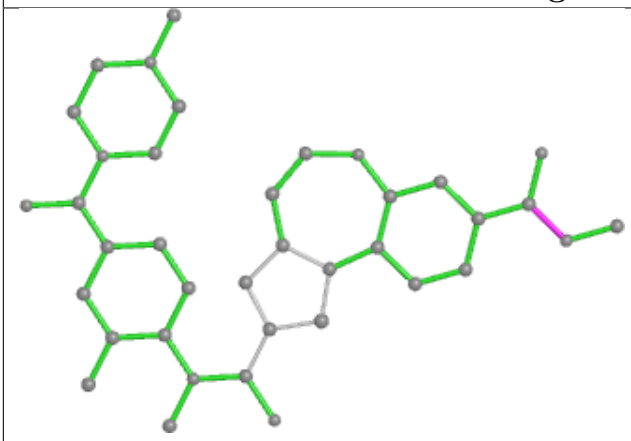
There are no ring outliers.

1 monomer is involved in 3 short contacts:

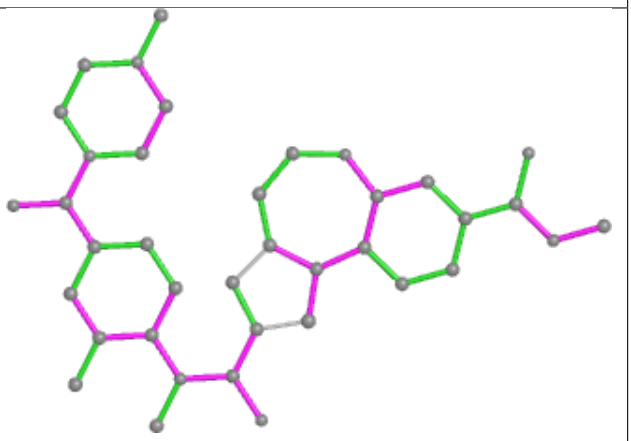
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	3T8	3	0

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.

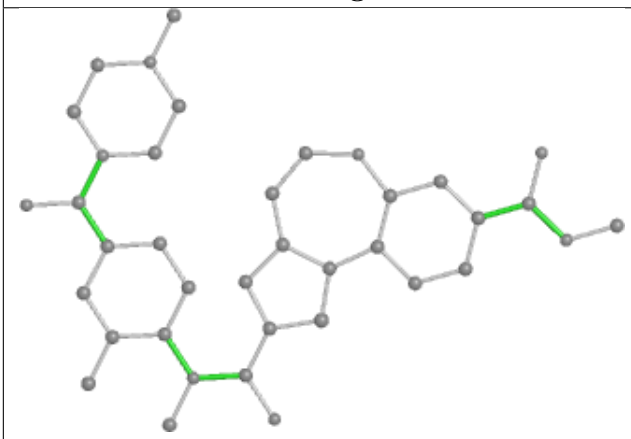
Ligand 3T8 A 1



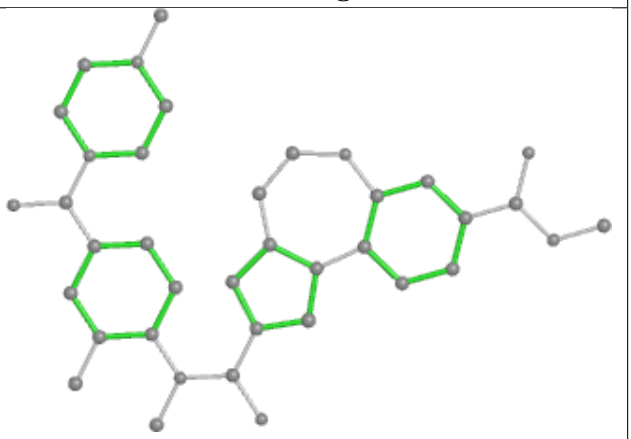
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	841/966 (87%)	0.46	94 (11%)	5 4	47, 97, 180, 235	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	19.5
1	A	1044	SER	12.7
1	A	375	ARG	10.4
1	A	544	ARG	8.8
1	A	377	THR	8.7
1	A	1086	TRP	8.5
1	A	376	ASN	8.1
1	A	896	VAL	6.7
1	A	1000	LYS	6.6
1	A	757	TYR	6.0
1	A	823	LEU	5.7
1	A	253	ALA	5.7
1	A	752	LEU	5.6
1	A	216	ALA	5.6
1	A	1091	VAL	5.4
1	A	374	PRO	5.3
1	A	143	MET	5.3
1	A	250	THR	5.2
1	A	373	LEU	5.2
1	A	378	ASP	5.2
1	A	981	GLU	5.0
1	A	322	GLU	5.0
1	A	545	ALA	4.9
1	A	998	SER	4.9
1	A	489	GLY	4.9
1	A	320	LYS	4.8
1	A	1084	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	755	GLU	4.5
1	A	898	ASN	4.3
1	A	1041	GLN	4.2
1	A	267	GLU	4.1
1	A	148	GLN	4.0
1	A	825	ASN	3.9
1	A	1090	LEU	3.8
1	A	252	MET	3.7
1	A	777	SER	3.6
1	A	1062	GLU	3.6
1	A	1042	LEU	3.5
1	A	270	PHE	3.5
1	A	916	PRO	3.4
1	A	315	LEU	3.3
1	A	1089	HIS	3.2
1	A	217	ASN	3.2
1	A	1046	GLU	3.2
1	A	832	PHE	3.1
1	A	999	GLY	3.0
1	A	899	THR	2.9
1	A	751	SER	2.8
1	A	213	LYS	2.8
1	A	993	PHE	2.8
1	A	429	LEU	2.8
1	A	982	ARG	2.8
1	A	756	LYS	2.8
1	A	269	ASP	2.7
1	A	488	SER	2.7
1	A	967	HIS	2.6
1	A	991	PHE	2.6
1	A	300	GLY	2.6
1	A	152	ARG	2.5
1	A	894	SER	2.5
1	A	749	ILE	2.5
1	A	549	ASN	2.4
1	A	834	HIS	2.4
1	A	909	HIS	2.4
1	A	1087	PHE	2.4
1	A	1007	GLN	2.4
1	A	229	THR	2.4
1	A	987	LEU	2.4
1	A	249	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	147	SER	2.4
1	A	754	ALA	2.3
1	A	919	GLU	2.3
1	A	895	THR	2.3
1	A	431	LEU	2.3
1	A	527	ILE	2.3
1	A	1043	THR	2.3
1	A	1001	LYS	2.3
1	A	717	LEU	2.3
1	A	234	LYS	2.3
1	A	613	ARG	2.2
1	A	550	GLN	2.2
1	A	246	GLN	2.2
1	A	1088	LEU	2.2
1	A	589	TYR	2.2
1	A	268	GLN	2.2
1	A	228	THR	2.2
1	A	359	ARG	2.2
1	A	932	CYS	2.1
1	A	997	THR	2.1
1	A	209	GLU	2.1
1	A	1015	LYS	2.0
1	A	546	GLU	2.0
1	A	988	THR	2.0
1	A	996	GLY	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)

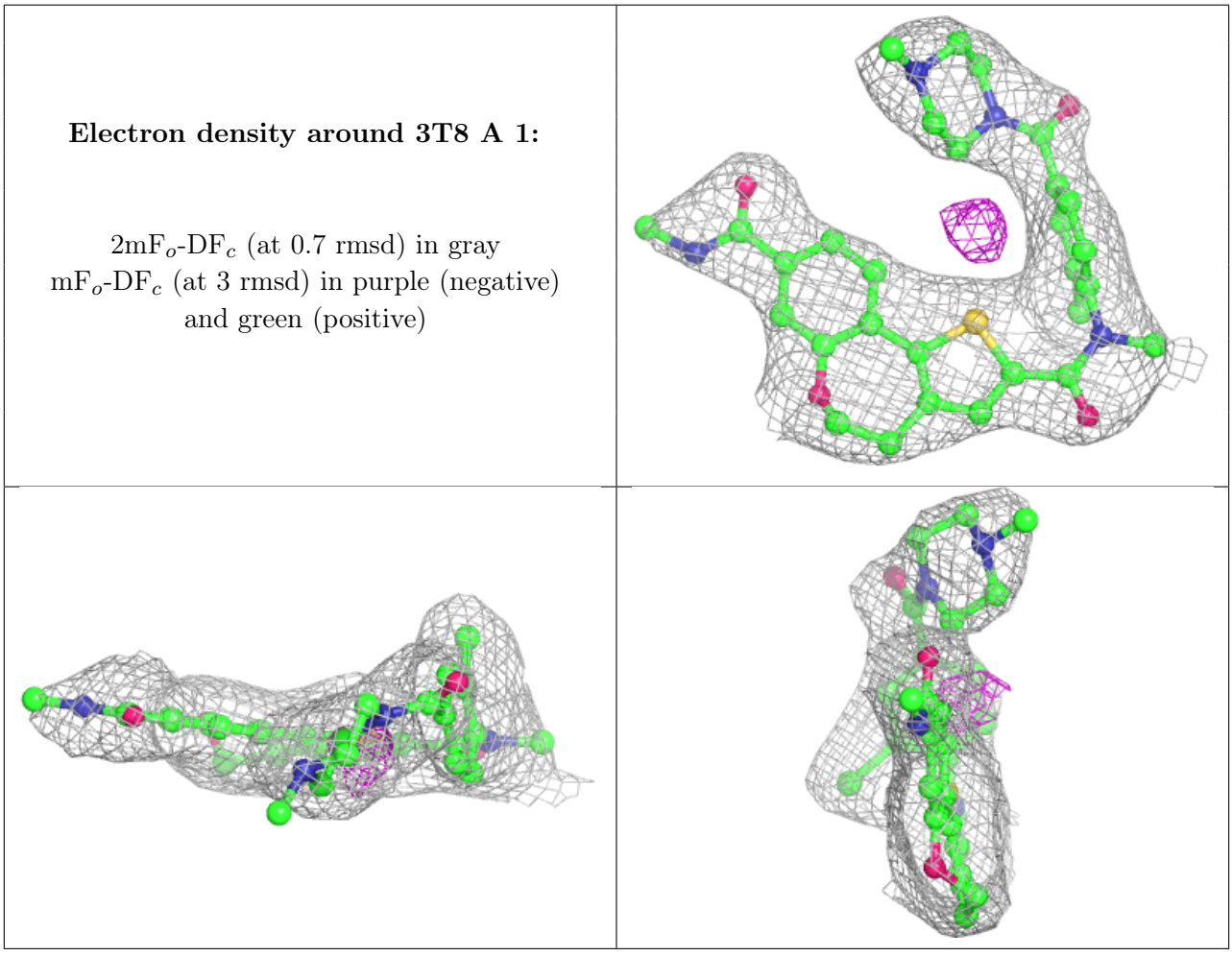
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	3T8	A	1	38/38	0.95	0.15	63,85,109,116	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 3T8 A 1:

$2mF_o$-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.