Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 07:01 am BST

PDB ID	:	5G55
Title	:	3-Quinoline Carboxamides inhibitors of Pi3K
Authors	:	Edman, K.; Phillips, C.
Deposited on	:	2016-05-20
Resolution	:	2.45 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:

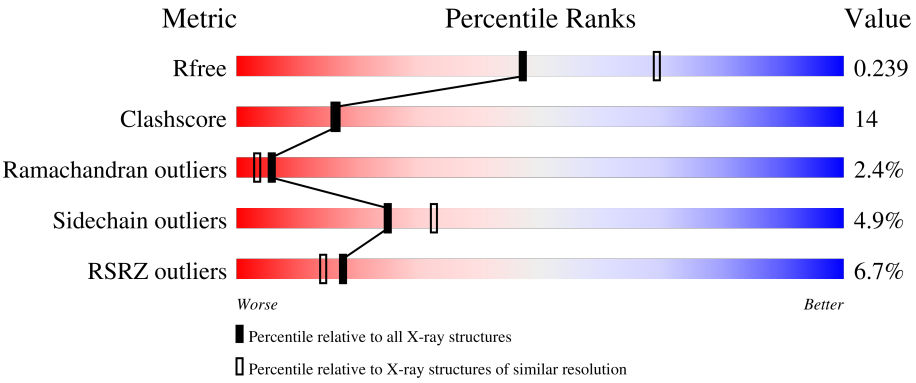
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	6% 62% 23% · 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6951 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.

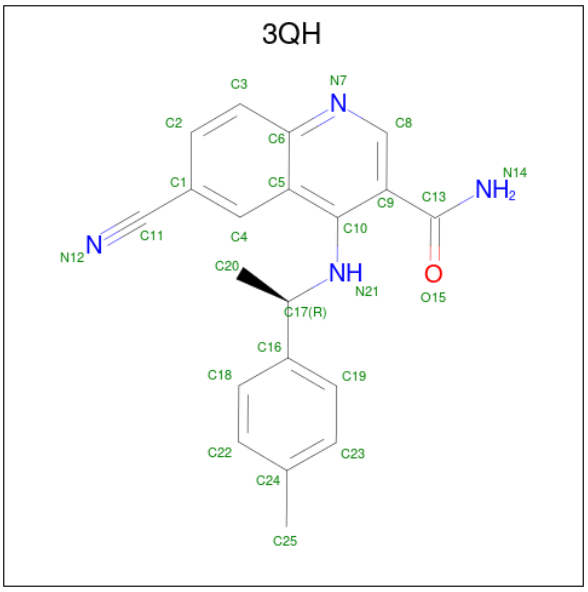
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	847	6877	4414	1175	1252	36	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

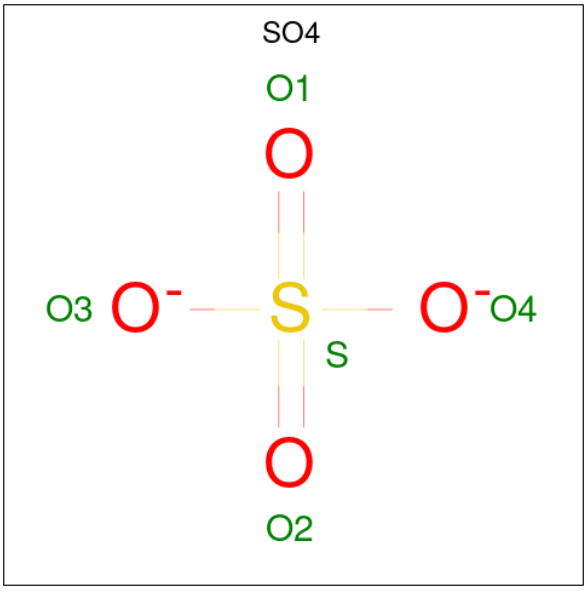
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736
A	268	ARG	GLN	conflict	UNP P48736

- Molecule 2 is 6-cyano-4-[[(1R)-1-(4-methylphenyl)ethyl]amino]quinoline-3-carboxamide (three-letter code: 3QH) (formula: $C_{20}H_{18}N_4O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 25 20 4 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

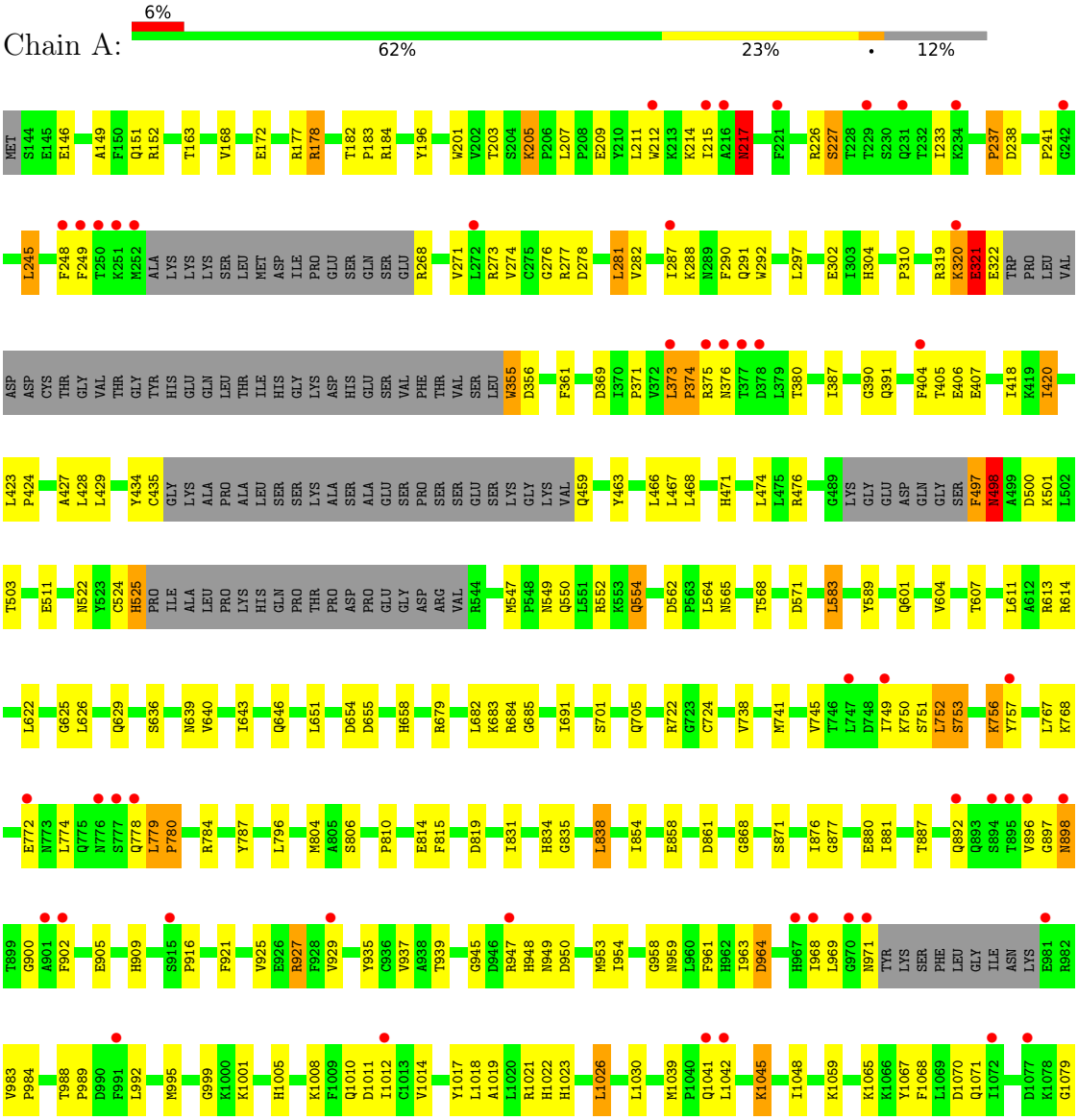
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0

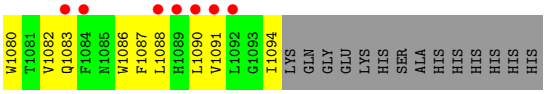
3 Residue-property plots (i)

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:




W1080
T1081
V1082
Q1083
F1084
N1085
W1086
F1087
L1088
H1089
L1090
V1091
L1092
G1093
I1094
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	140.08Å 67.18Å 104.56Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	72.00 – 2.45 44.14 – 2.24	Depositor EDS
% Data completeness (in resolution range)	96.2 (72.00-2.45) 99.5 (44.14-2.24)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.254 , 0.322 0.251 , 0.239	Depositor DCC
R_{free} test set	2301 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6951	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: SO4, 3QH

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	0.60	0/7026	0.79	6/9505 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	428	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	245	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	583	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	779	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	474	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	684	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	6877	0	6910	196	0
2	A	25	0	0	4	0
3	A	5	0	0	0	0
4	A	44	0	0	2	0
All	All	6951	0	6910	198	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 14.

All (198) 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:320:LYS:HA	1:A:321:GLU:HB3	1.23	1.15
1:A:927:ARG:HH11	1:A:927:ARG:HG3	1.11	1.09
1:A:896:VAL:HG23	1:A:897:GLY:H	1.25	0.99
1:A:373:LEU:H	1:A:374:PRO:HD2	1.29	0.95
1:A:1045:LYS:H	1:A:1045:LYS:HD2	1.32	0.92
1:A:498:ASN:HD22	1:A:500:ASP:H	1.21	0.87
1:A:927:ARG:HG3	1:A:927:ARG:NH1	1.92	0.85
1:A:184:ARG:HD3	4:A:2009:HOH:O	1.77	0.84
1:A:524:CYS:HB3	1:A:525:HIS:HB3	1.58	0.83
1:A:927:ARG:HH11	1:A:927:ARG:CG	1.90	0.83
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.61	0.82
1:A:524:CYS:HB3	1:A:525:HIS:CB	2.08	0.82
1:A:434:TYR:HA	1:A:459:GLN:O	1.82	0.79
1:A:498:ASN:ND2	1:A:500:ASP:H	1.81	0.79
1:A:947:ARG:NH2	1:A:963:ILE:O	2.16	0.78
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.50	0.76
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.85	0.75
1:A:163:THR:HG22	1:A:177:ARG:NH1	2.02	0.75
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.52	0.74
1:A:896:VAL:HG23	1:A:897:GLY:N	2.02	0.73
1:A:898:ASN:N	1:A:898:ASN:HD22	1.85	0.73
1:A:1045:LYS:H	1:A:1045:LYS:CD	2.01	0.73
1:A:524:CYS:HB3	1:A:525:HIS:CA	2.20	0.72
1:A:750:LYS:HG2	1:A:751:SER:H	1.55	0.72
1:A:625:GLY:O	1:A:629:GLN:HG3	1.90	0.72
1:A:320:LYS:HA	1:A:321:GLU:CB	2.12	0.71
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.38	0.71
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.37	0.70
1:A:371:PRO:HG2	1:A:511:GLU:O	1.91	0.69
1:A:146:GLU:HG3	1:A:319:ARG:HH21	1.57	0.69
1:A:614:ARG:HH11	1:A:646:GLN:NE2	1.92	0.67
1:A:896:VAL:CG2	1:A:897:GLY:H	2.02	0.67
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.76	0.66
1:A:497:PHE:O	1:A:498:ASN:HB2	1.96	0.65
1:A:947:ARG:HD3	1:A:968:ILE:HD13	1.79	0.65
1:A:233:ILE:CD1	1:A:248:PHE:HD1	2.09	0.64
1:A:905:GLU:HB3	1:A:909:HIS:NE2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:HB	1:A:183:PRO:HD3	1.81	0.63
1:A:466:LEU:HD21	1:A:476:ARG:HD3	1.81	0.62
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.34	0.61
1:A:898:ASN:O	1:A:1087:PHE:HZ	1.84	0.61
1:A:892:GLN:O	1:A:896:VAL:HG22	2.01	0.61
1:A:654:ASP:O	1:A:658:HIS:HD2	1.84	0.60
1:A:898:ASN:HD22	1:A:898:ASN:H	1.48	0.60
1:A:954:ILE:HG13	1:A:959:ASN:O	2.03	0.59
1:A:992:LEU:HD23	1:A:995:MET:CE	2.32	0.59
1:A:549:ASN:O	1:A:552:ARG:HB3	2.03	0.58
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.04	0.58
1:A:373:LEU:N	1:A:374:PRO:HD2	2.09	0.58
1:A:196:TYR:OH	1:A:724:CYS:O	2.17	0.58
1:A:995:MET:O	1:A:1005:HIS:HB2	2.03	0.58
1:A:497:PHE:O	1:A:498:ASN:CB	2.51	0.57
1:A:701:SER:O	1:A:705:GLN:HG2	2.03	0.57
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.86	0.57
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.05	0.57
1:A:858:GLU:HG3	1:A:1019:ALA:HB1	1.85	0.56
1:A:898:ASN:N	1:A:898:ASN:ND2	2.52	0.56
1:A:320:LYS:N	1:A:320:LYS:HD3	2.21	0.56
1:A:302:GLU:HB2	1:A:304:HIS:NE2	2.22	0.55
1:A:276:GLY:HA2	1:A:819:ASP:CG	2.26	0.55
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.40	0.55
1:A:373:LEU:H	1:A:374:PRO:CD	2.11	0.54
1:A:939:THR:HB	1:A:945:GLY:HA2	1.88	0.54
1:A:217:ASN:HD22	1:A:217:ASN:C	2.10	0.54
1:A:774:LEU:O	1:A:778:GLN:HB3	2.07	0.54
1:A:749:ILE:HG12	1:A:767:LEU:HA	1.90	0.53
1:A:925:VAL:O	1:A:929:VAL:HG23	2.07	0.53
1:A:183:PRO:HB3	1:A:683:LYS:HE2	1.89	0.53
1:A:226:ARG:O	1:A:227:SER:C	2.46	0.53
1:A:463:TYR:CE2	1:A:501:LYS:HA	2.43	0.53
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.43	0.53
1:A:183:PRO:HB3	1:A:683:LYS:CE	2.39	0.53
1:A:963:ILE:HD12	1:A:964:ASP:HB2	1.91	0.53
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.90	0.53
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.91	0.53
1:A:640:VAL:O	1:A:643:ILE:HG12	2.09	0.52
1:A:375:ARG:HE	1:A:376:ASN:ND2	2.08	0.52
1:A:212:TRP:C	1:A:214:LYS:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:HG3	1:A:319:ARG:NH2	2.25	0.52
1:A:1082:VAL:HG12	1:A:1086:TRP:CD1	2.44	0.52
1:A:750:LYS:HG2	1:A:751:SER:N	2.23	0.52
1:A:1041:GLN:HG2	1:A:1042:LEU:H	1.75	0.52
1:A:420:ILE:HD13	1:A:522:ASN:HB3	1.92	0.51
1:A:201:TRP:CE2	1:A:291:GLN:HG2	2.46	0.51
1:A:804:MET:HB2	1:A:810:PRO:HG2	1.93	0.51
1:A:1041:GLN:HG2	1:A:1042:LEU:N	2.25	0.51
1:A:498:ASN:HD22	1:A:500:ASP:N	1.99	0.51
1:A:245:LEU:O	1:A:249:PHE:HB2	2.11	0.51
1:A:550:GLN:NE2	1:A:554:GLN:OE1	2.43	0.51
1:A:320:LYS:HD3	1:A:320:LYS:H	1.76	0.51
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.38	0.51
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.10	0.51
1:A:768:LYS:O	1:A:772:GLU:HB2	2.11	0.50
1:A:834:HIS:HB2	1:A:876:ILE:HG22	1.92	0.50
1:A:622:LEU:HD21	1:A:651:LEU:HG	1.91	0.50
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.46	0.50
1:A:380:THR:O	1:A:435:CYS:HB2	2.11	0.50
1:A:831:ILE:HD13	2:A:2095:3QH:C23	2.42	0.50
1:A:751:SER:O	1:A:752:LEU:CD2	2.60	0.49
1:A:1022:HIS:CD2	4:A:2044:HOH:O	2.65	0.49
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.95	0.49
1:A:738:VAL:HG23	1:A:780:PRO:HG2	1.93	0.49
1:A:207:LEU:CD2	1:A:211:LEU:HB2	2.42	0.49
1:A:927:ARG:NH1	1:A:927:ARG:CG	2.62	0.49
1:A:214:LYS:HD2	1:A:297:LEU:O	2.12	0.49
1:A:245:LEU:HA	1:A:249:PHE:HD1	1.78	0.49
1:A:992:LEU:HA	1:A:995:MET:HE3	1.94	0.49
1:A:1041:GLN:HG2	1:A:1042:LEU:HD12	1.94	0.49
1:A:500:ASP:O	1:A:503:THR:HG22	2.12	0.48
1:A:524:CYS:CB	1:A:525:HIS:CA	2.91	0.48
1:A:497:PHE:HB3	1:A:501:LYS:HE2	1.96	0.48
1:A:750:LYS:NZ	1:A:834:HIS:CD2	2.81	0.48
1:A:1091:VAL:HG12	1:A:1091:VAL:O	2.13	0.48
1:A:861:ASP:OD1	1:A:861:ASP:C	2.52	0.48
1:A:937:VAL:HG22	1:A:1068:PHE:CZ	2.49	0.48
1:A:201:TRP:CZ2	1:A:291:GLN:HG2	2.49	0.48
1:A:988:THR:HB	1:A:989:PRO:HD2	1.96	0.48
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.47	0.47
1:A:149:ALA:HA	1:A:152:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:TRP:HE3	1:A:1090:LEU:HD13	1.77	0.47
1:A:752:LEU:O	1:A:753:SER:HB3	2.13	0.47
1:A:787:TYR:CE1	1:A:880:GLU:HB2	2.49	0.47
1:A:547:MET:HB3	1:A:552:ARG:HH11	1.80	0.47
1:A:949:ASN:N	1:A:1083:GLN:HE22	2.10	0.47
1:A:887:THR:HA	1:A:953:MET:HG2	1.97	0.47
1:A:361:PHE:CD2	1:A:387:ILE:HD11	2.50	0.46
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.12	0.46
1:A:948:HIS:CD2	1:A:950:ASP:H	2.33	0.46
1:A:562:ASP:OD1	1:A:565:ASN:HB2	2.15	0.46
1:A:921:PHE:O	1:A:925:VAL:HG23	2.16	0.46
1:A:390:GLY:N	1:A:636:SER:OG	2.49	0.46
1:A:568:THR:HG23	1:A:571:ASP:H	1.81	0.46
1:A:927:ARG:HD3	1:A:959:ASN:HB2	1.97	0.45
1:A:203:THR:OG1	1:A:205:LYS:NZ	2.49	0.45
1:A:750:LYS:HZ3	1:A:834:HIS:CD2	2.34	0.45
1:A:963:ILE:HB	2:A:2095:3QH:C11	2.46	0.45
1:A:834:HIS:CG	1:A:835:GLY:N	2.85	0.45
1:A:779:LEU:HD21	1:A:796:LEU:HD12	1.97	0.45
1:A:992:LEU:HD23	1:A:995:MET:HE1	1.97	0.45
1:A:614:ARG:NH1	1:A:646:GLN:NE2	2.63	0.45
1:A:838:LEU:CD2	1:A:877:GLY:HA3	2.46	0.45
1:A:524:CYS:HB3	1:A:525:HIS:HA	1.95	0.45
1:A:524:CYS:CB	1:A:525:HIS:HA	2.47	0.45
1:A:831:ILE:HG13	1:A:881:ILE:HG12	1.99	0.45
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.82	0.44
1:A:787:TYR:CD1	1:A:868:GLY:HA3	2.52	0.44
1:A:968:ILE:HG13	1:A:969:LEU:N	2.33	0.44
1:A:989:PRO:HG2	1:A:1080:TRP:NE1	2.32	0.44
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.18	0.44
1:A:178:ARG:HG2	1:A:178:ARG:HH11	1.83	0.44
1:A:320:LYS:CA	1:A:321:GLU:HB3	2.17	0.44
1:A:273:ARG:NH1	1:A:277:ARG:O	2.49	0.44
1:A:287:ILE:HD12	1:A:288:LYS:N	2.33	0.44
1:A:424:PRO:HG2	1:A:427:ALA:HB2	1.99	0.44
1:A:1041:GLN:CG	1:A:1042:LEU:H	2.30	0.44
1:A:954:ILE:HG13	1:A:959:ASN:C	2.38	0.43
1:A:418:ILE:HD13	1:A:423:LEU:HD23	2.00	0.43
1:A:420:ILE:CD1	1:A:522:ASN:HB3	2.48	0.43
1:A:948:HIS:CD2	1:A:950:ASP:HB2	2.53	0.43
1:A:954:ILE:HA	1:A:959:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:HH11	1:A:968:ILE:HG23	1.82	0.43
1:A:355:TRP:HB2	1:A:356:ASP:H	1.64	0.43
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.33	0.43
1:A:497:PHE:HB3	1:A:501:LYS:CE	2.49	0.43
1:A:679:ARG:HB3	1:A:683:LYS:HE3	2.01	0.43
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.54	0.43
1:A:604:VAL:O	1:A:607:THR:HB	2.18	0.43
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.54	0.42
1:A:900:GLY:HA2	1:A:902:PHE:CZ	2.54	0.42
1:A:992:LEU:HD23	1:A:995:MET:HE3	2.01	0.42
1:A:1088:LEU:HB3	1:A:1094:ILE:HG13	2.01	0.42
1:A:679:ARG:O	1:A:683:LYS:HG3	2.19	0.42
1:A:271:VAL:HG23	1:A:310:PRO:HD3	2.02	0.42
1:A:241:PRO:HB3	1:A:281:LEU:O	2.20	0.42
1:A:467:LEU:O	1:A:476:ARG:NH1	2.49	0.42
1:A:583:LEU:HD12	1:A:589:TYR:OH	2.20	0.42
1:A:207:LEU:HD21	1:A:211:LEU:HB2	2.01	0.42
1:A:1067:TYR:O	1:A:1070:ASP:HB2	2.20	0.41
1:A:756:LYS:HG3	1:A:757:TYR:H	1.84	0.41
2:A:2095:3QH:O15	2:A:2095:3QH:N21	2.52	0.41
1:A:796:LEU:HG	1:A:815:PHE:CE2	2.56	0.41
1:A:568:THR:HG22	1:A:571:ASP:CG	2.40	0.41
2:A:2095:3QH:C17	2:A:2095:3QH:C4	2.99	0.41
1:A:320:LYS:O	1:A:320:LYS:HG2	2.21	0.41
1:A:405:THR:OG1	1:A:407:GLU:O	2.38	0.41
1:A:639:ASN:O	1:A:643:ILE:HG23	2.20	0.41
1:A:701:SER:HB2	1:A:871:SER:OG	2.21	0.41
1:A:741:MET:CE	1:A:778:GLN:HG3	2.51	0.41
1:A:751:SER:O	1:A:752:LEU:HD22	2.21	0.41
1:A:905:GLU:HB3	1:A:909:HIS:CD2	2.55	0.41
1:A:745:VAL:O	1:A:749:ILE:HD13	2.21	0.41
1:A:1021:ARG:C	1:A:1023:HIS:H	2.25	0.41
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.51	0.40
1:A:779:LEU:HA	1:A:780:PRO:HD2	1.84	0.40
1:A:611:LEU:O	1:A:614:ARG:HB2	2.21	0.40
1:A:896:VAL:CG2	1:A:897:GLY:N	2.71	0.40
1:A:390:GLY:O	1:A:391:GLN:HB2	2.22	0.40
1:A:954:ILE:HD11	1:A:958:GLY:HA2	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	833/966 (86%)	727 (87%)	86 (10%)	20 (2%)	6 3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	321	GLU
1	A	373	LEU
1	A	498	ASN
1	A	753	SER
1	A	806	SER
1	A	916	PRO
1	A	752	LEU
1	A	999	GLY
1	A	1001	LYS
1	A	1079	GLY
1	A	613	ARG
1	A	756	LYS
1	A	780	PRO
1	A	217	ASN
1	A	984	PRO
1	A	237	PRO
1	A	420	ILE
1	A	215	ILE
1	A	374	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	762/864 (88%)	725 (95%)	37 (5%)	25 32

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	VAL
1	A	178	ARG
1	A	205	LYS
1	A	209	GLU
1	A	217	ASN
1	A	238	ASP
1	A	268	ARG
1	A	278	ASP
1	A	281	LEU
1	A	282	VAL
1	A	320	LYS
1	A	321	GLU
1	A	322	GLU
1	A	355	TRP
1	A	369	ASP
1	A	404	PHE
1	A	406	GLU
1	A	497	PHE
1	A	498	ASN
1	A	525	HIS
1	A	554	GLN
1	A	601	GLN
1	A	626	LEU
1	A	682	LEU
1	A	784	ARG
1	A	814	GLU
1	A	838	LEU
1	A	898	ASN
1	A	927	ARG
1	A	964	ASP
1	A	971	ASN
1	A	983	VAL
1	A	1011	ASP
1	A	1026	LEU
1	A	1039	MET
1	A	1045	LYS

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Mol	Chain	Res	Type
1	A	1059	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	376	ASN
1	A	392	GLN
1	A	486	GLN
1	A	498	ASN
1	A	601	GLN
1	A	646	GLN
1	A	658	HIS
1	A	710	GLN
1	A	743	GLN
1	A	834	HIS
1	A	840	GLN
1	A	892	GLN
1	A	898	ASN
1	A	948	HIS
1	A	951	ASN
1	A	971	ASN
1	A	1023	HIS
1	A	1083	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	2096	-	4,4,4	0.16	0	6,6,6	0.28	0
2	3QH	A	2095	-	27,27,27	0.75	1 (3%)	33,38,38	1.54	7 (21%)

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	3QH	A	2095	-	-	2/14/14/14	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	3QH	C13-N14	2.18	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2095	3QH	C8-N7-C6	4.28	122.07	116.91
2	A	2095	3QH	O15-C13-N14	-3.34	117.84	122.58
2	A	2095	3QH	C4-C1-C11	2.60	121.90	119.65
2	A	2095	3QH	C16-C17-N21	-2.32	107.81	112.56
2	A	2095	3QH	C9-C13-N14	2.25	121.75	118.29
2	A	2095	3QH	C9-C8-N7	-2.14	122.25	125.14
2	A	2095	3QH	C4-C5-C10	2.08	125.77	123.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2095	3QH	C5-C10-N21-C17
2	A	2095	3QH	C9-C10-N21-C17

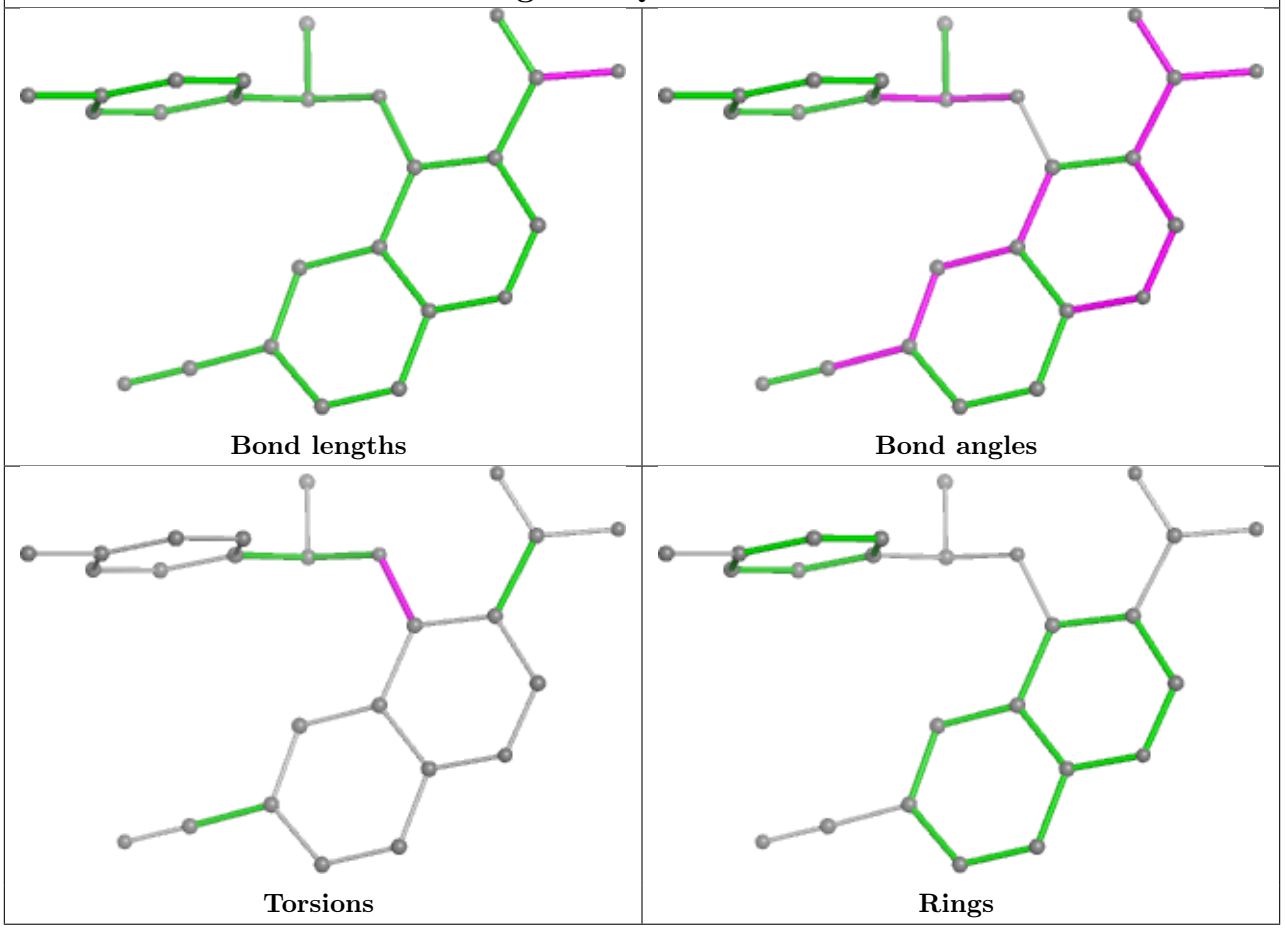
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2095	3QH	4	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 3QH A 2095



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	847/966 (87%)	0.37	57 (6%)	17	14	15, 48, 77, 94	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	968	ILE	7.0
1	A	215	ILE	6.8
1	A	375	ARG	5.4
1	A	376	ASN	5.4
1	A	1084	PHE	5.3
1	A	216	ALA	4.9
1	A	287	ILE	4.7
1	A	249	PHE	4.6
1	A	378	ASP	4.3
1	A	1088	LEU	4.2
1	A	776	ASN	4.2
1	A	757	TYR	4.1
1	A	221	PHE	4.0
1	A	971	ASN	3.9
1	A	1090	LEU	3.8
1	A	212	TRP	3.6
1	A	1092	LEU	3.5
1	A	902	PHE	3.5
1	A	967	HIS	3.3
1	A	895	THR	3.2
1	A	1091	VAL	3.2
1	A	749	ILE	3.2
1	A	915	SER	3.1
1	A	248	PHE	3.0
1	A	373	LEU	3.0
1	A	1089	HIS	2.9
1	A	1083	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	981	GLU	2.7
1	A	252	MET	2.7
1	A	251	LYS	2.6
1	A	404	PHE	2.6
1	A	377	THR	2.6
1	A	898	ASN	2.6
1	A	250	THR	2.6
1	A	320	LYS	2.6
1	A	778	GLN	2.5
1	A	234	LYS	2.5
1	A	229	THR	2.5
1	A	1077	ASP	2.4
1	A	1041	GLN	2.4
1	A	777	SER	2.4
1	A	929	VAL	2.4
1	A	894	SER	2.4
1	A	242	GLY	2.3
1	A	947	ARG	2.3
1	A	1042	LEU	2.3
1	A	901	ALA	2.3
1	A	231	GLN	2.3
1	A	896	VAL	2.3
1	A	1012	ILE	2.3
1	A	272	LEU	2.2
1	A	892	GLN	2.2
1	A	991	PHE	2.2
1	A	970	GLY	2.1
1	A	1072	ILE	2.0
1	A	747	LEU	2.0
1	A	772	GLU	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)

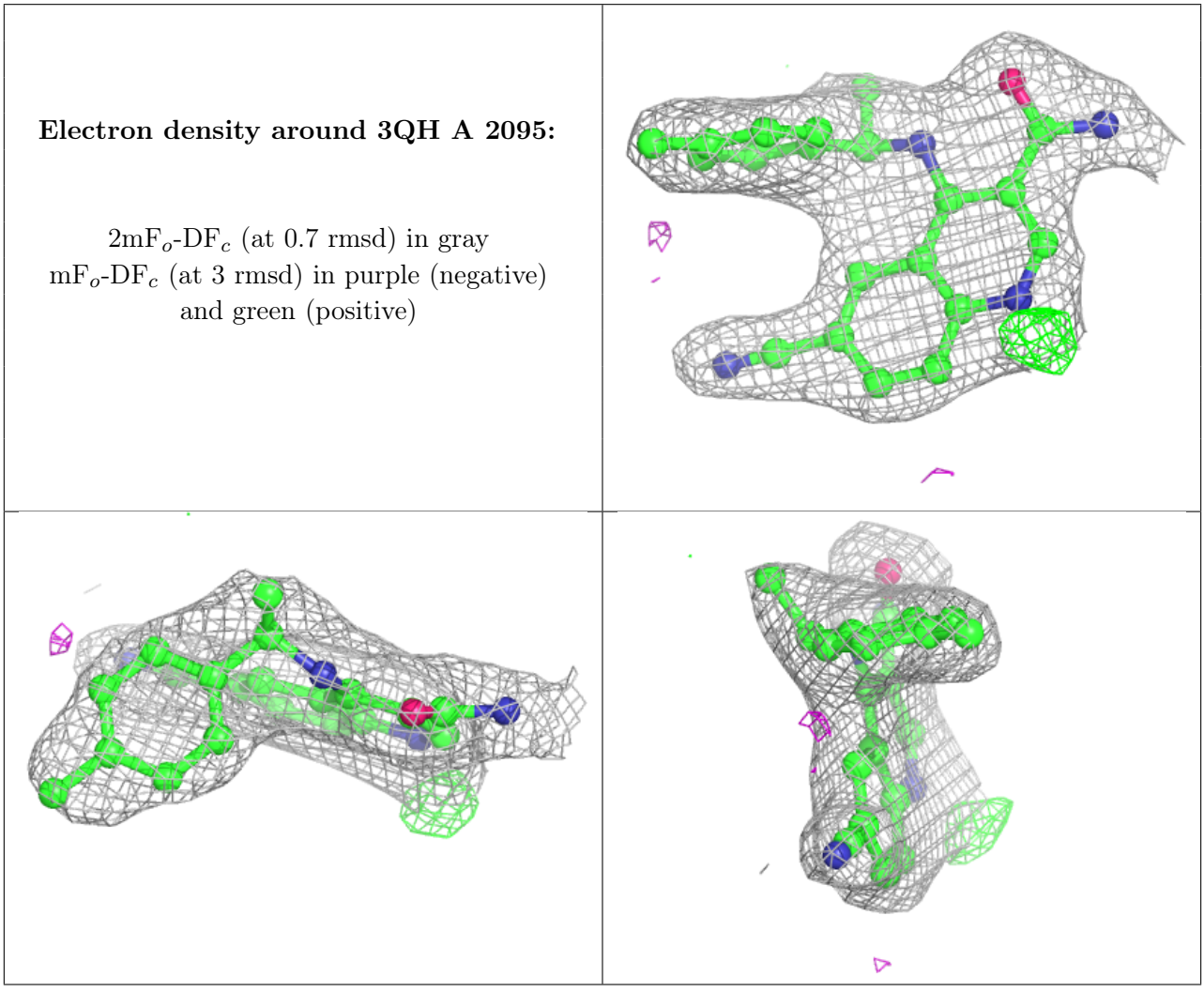
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	3QH	A	2095	25/25	0.92	0.14	37,39,41,41	0
3	SO4	A	2096	5/5	0.94	0.07	79,79,80,81	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 3QH A 2095:

$2mF_o$-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.