



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:14 AM UTC

PDB ID : 5G55 / pdb_00005g55
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

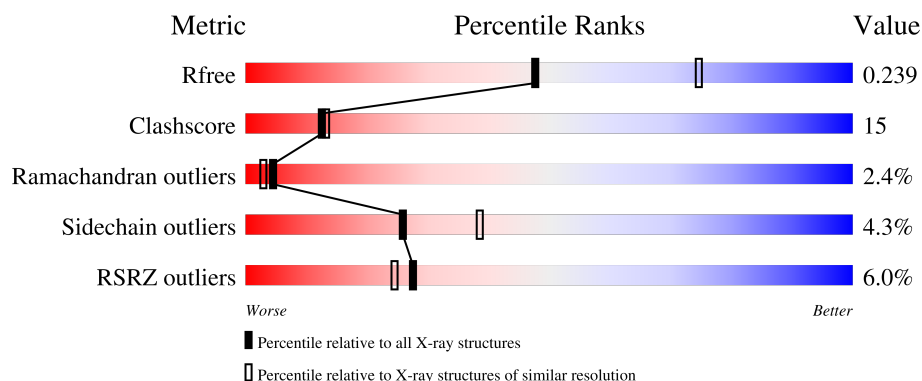
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 $\leq 5\%$. 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	5% 59% 25% • 12%

2 Entry composition

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.

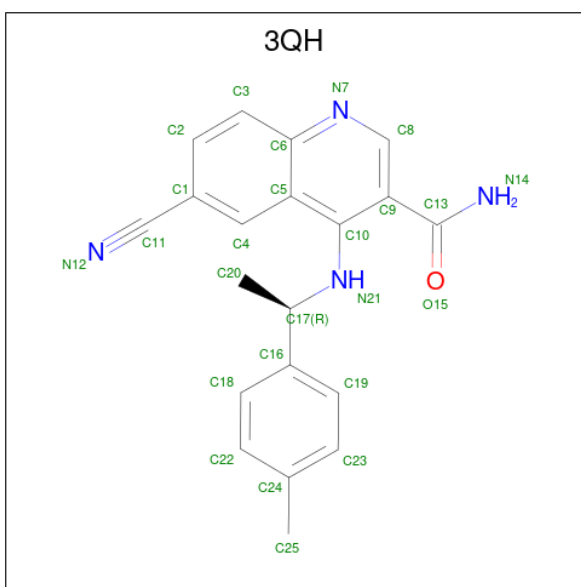
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

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

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 (CCD ID: 3QH) (formula: C₂₀H₁₈N₄O).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

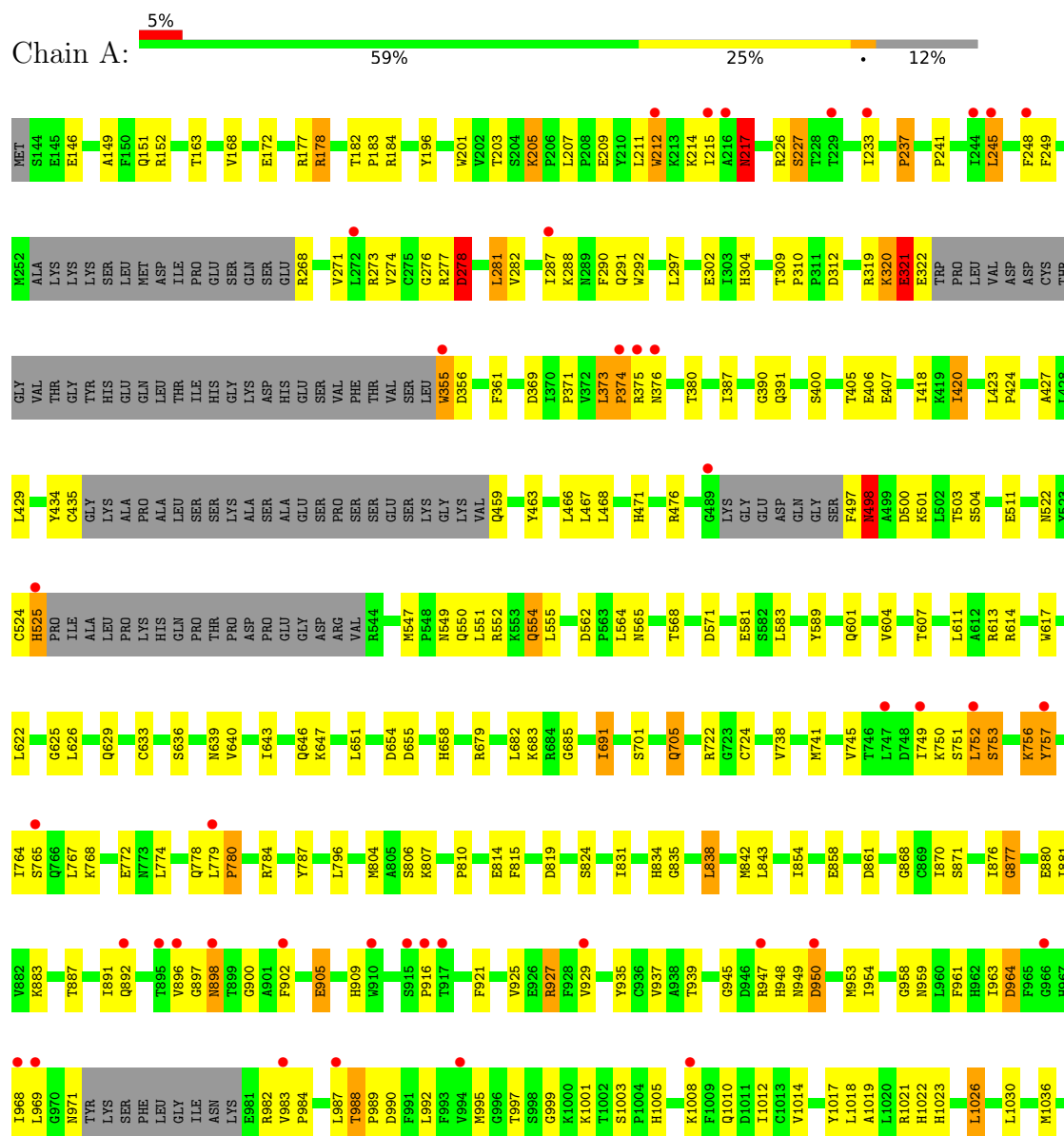
- Molecule 4 is water.

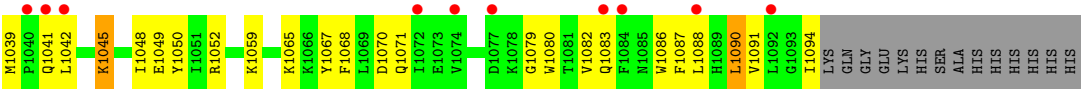
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0

3 Residue-property plots

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 SUB-UNIT GAMMA ISOFORM





4 Data and refinement statistics

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 72.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.2 (72.00-2.45) 99.7 (72.00-2.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 3QH, SO4

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	0.73	0/7026	1.10	28/9505 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	LEU	N-CA-C	-10.75	101.20	114.75
1	A	807	LYS	N-CA-C	9.29	121.01	111.07
1	A	982	ARG	N-CA-C	7.41	118.05	108.34
1	A	824	SER	N-CA-C	7.29	117.59	108.19
1	A	905	GLU	N-CA-C	7.18	118.89	111.14
1	A	1090	LEU	N-CA-C	6.04	118.77	111.40
1	A	757	TYR	N-CA-C	6.04	118.13	108.41
1	A	400	SER	N-CA-C	-6.00	101.57	110.20
1	A	877	GLY	N-CA-C	5.88	119.09	110.38
1	A	691	ILE	N-CA-C	-5.71	104.95	110.72
1	A	504	SER	N-CA-C	-5.69	106.33	113.28
1	A	212	TRP	N-CA-C	-5.68	105.08	112.23
1	A	312	ASP	CA-C-N	5.47	125.14	119.56
1	A	312	ASP	C-N-CA	5.47	125.14	119.56
1	A	320	LYS	N-CA-C	5.41	116.27	107.23
1	A	1003	SER	N-CA-C	5.40	114.51	108.25
1	A	988	THR	CA-C-N	5.38	125.45	119.32
1	A	988	THR	C-N-CA	5.38	125.45	119.32
1	A	278	ASP	N-CA-C	-5.38	103.87	110.65
1	A	950	ASP	N-CA-C	-5.37	106.23	112.89
1	A	309	THR	CA-C-N	5.23	125.77	120.38
1	A	309	THR	C-N-CA	5.23	125.77	120.38
1	A	883	LYS	N-CA-C	5.22	121.92	110.80
1	A	891	ILE	N-CA-C	-5.19	104.49	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	997	THR	N-CA-C	5.11	116.83	109.07
1	A	320	LYS	CA-C-N	5.09	130.86	121.70
1	A	320	LYS	C-N-CA	5.09	130.86	121.70
1	A	581	GLU	N-CA-C	-5.06	105.22	111.40

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	209	0
2	A	25	0	0	5	0
3	A	5	0	0	0	0
4	A	44	0	0	2	0
All	All	6951	0	6910	211	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 (211) 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:HG3	1:A:927:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:547:MET:HE1	1:A:555:LEU:HB2	1.82	0.61
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:276:GLY:HA2	1:A:819:ASP:CG	2.26	0.59
1:A:954:ILE:HG13	1:A:959:ASN:O	2.03	0.59
1:A:217:ASN:C	1:A:217:ASN:HD22	2.10	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:226:ARG:O	1:A:227:SER:C	2.46	0.58
1:A:373:LEU:N	1:A:374:PRO:HD2	2.09	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:212:TRP:C	1:A:214:LYS:H	2.13	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:HD3	1:A:320:LYS:N	2.21	0.56
1:A:302:GLU:HB2	1:A:304:HIS:NE2	2.22	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: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: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:992:LEU:HD23	1:A:995:MET:HE3	1.91	0.53
1:A:183:PRO:HB3	1:A:683:LYS:CE	2.39	0.53
1:A:633:CYS:SG	1:A:1036:MET:HE1	2.49	0.53
1:A:861:ASP:OD1	1:A:861:ASP:C	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:987:LEU:HD11	1:A:995:MET:HE1	1.95	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: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:954:ILE:HG13	1:A:959:ASN:C	2.38	0.48
1:A:1091:VAL:HG12	1:A:1091:VAL:O	2.13	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
1:A:547:MET:HE2	1:A:551:LEU:C	2.40	0.47
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:617:TRP:O	1:A:647:LYS:NZ	2.48	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:568:THR:HG22	1:A:571:ASP:CG	2.40	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:842:MET:HE3	1:A:870:ILE:HD13	1.98	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:1021:ARG:C	1:A:1023:HIS:H	2.25	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: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:953:MET:HE1	2:A:2095:3QH:C9	2.47	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: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
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:1049:GLU:O	1:A:1050:TYR:C	2.61	0.43
1:A:990:ASP:CG	1:A:1080:TRP:HH2	2.27	0.43
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:ASP:CG	1:A:784:ARG:HH22	2.27	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:373:LEU:C	1:A:373:LEU:HD12	2.44	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:562:ASP:CG	1:A:1052:ARG:HH21	2.27	0.41
1:A:796:LEU:HG	1:A:815:PHE:CE2	2.56	0.41
2:A:2095:3QH:C4	2:A:2095:3QH:C17	2.99	0.41
1:A:320:LYS:HG2	1:A:320:LYS:O	2.21	0.41
1:A:405:THR:OG1	1:A:407:GLU:O	2.38	0.41
1:A:905:GLU:H	1:A:905:GLU:CD	2.28	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:237:PRO:HA	1:A:287:ILE:CD1	2.51	0.40
1:A:764:ILE:O	1:A:765:SER:C	2.63	0.40
1:A:779:LEU:HA	1:A:780:PRO:HD2	1.84	0.40
1:A:1050:TYR:C	1:A:1050:TYR:CD1	2.99	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%)	4 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%)	729 (96%)	33 (4%)	26	38

All (33) 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	268	ARG
1	A	278	ASP
1	A	281	LEU
1	A	282	VAL
1	A	321	GLU
1	A	322	GLU
1	A	355	TRP
1	A	369	ASP
1	A	406	GLU
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	705	GLN
1	A	814	GLU
1	A	838	LEU
1	A	843	LEU
1	A	898	ASN
1	A	927	ARG
1	A	964	ASP
1	A	971	ASN
1	A	983	VAL
1	A	1026	LEU
1	A	1039	MET
1	A	1045	LYS
1	A	1059	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	376	ASN
1	A	389	HIS
1	A	392	GLN
1	A	396	GLN
1	A	486	GLN
1	A	498	ASN
1	A	601	GLN
1	A	646	GLN
1	A	658	HIS
1	A	705	GLN
1	A	710	GLN
1	A	743	GLN
1	A	834	HIS
1	A	846	GLN
1	A	892	GLN
1	A	898	ASN
1	A	948	HIS
1	A	951	ASN
1	A	959	ASN
1	A	971	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 oligosaccharides 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
2	3QH	A	2095	-	26,27,27	0.78	1 (3%)	32,38,38	1.59	8 (25%)
3	SO4	A	2096	-	4,4,4	0.27	0	6,6,6	0.20	0

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	2.27	1.37	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2095	3QH	C8-N7-C6	4.41	122.07	116.96
2	A	2095	3QH	O15-C13-N14	-3.31	117.84	122.62
2	A	2095	3QH	C4-C1-C11	2.63	121.90	119.66
2	A	2095	3QH	C16-C17-N21	-2.50	107.81	112.53
2	A	2095	3QH	C9-C8-N7	-2.27	122.25	125.20
2	A	2095	3QH	C4-C5-C10	2.24	125.77	123.19
2	A	2095	3QH	C9-C13-N14	2.23	121.75	118.29
2	A	2095	3QH	C4-C5-C6	-2.05	116.58	118.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

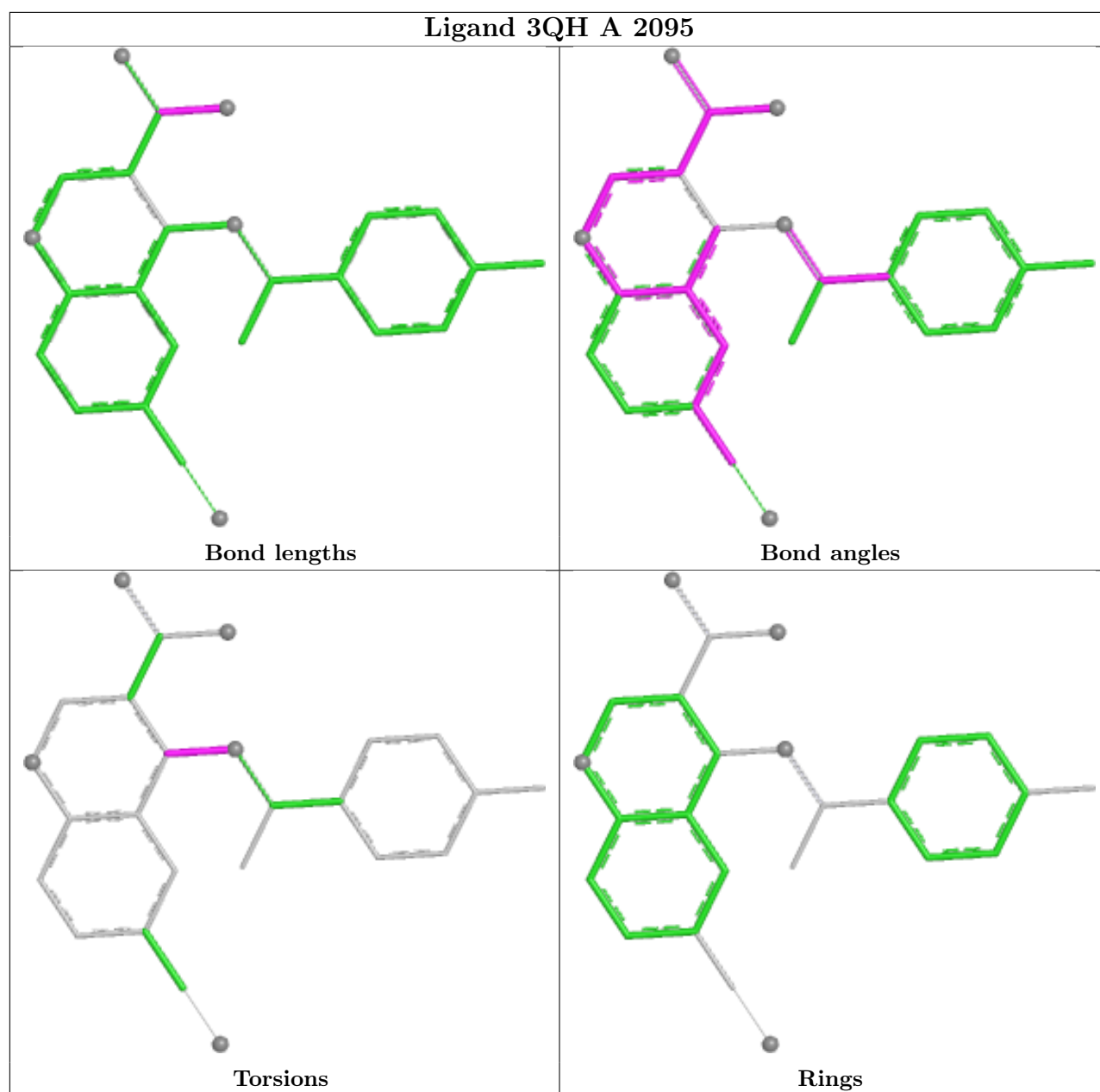
Mol	Chain	Res	Type	Atoms
2	A	2095	3QH	C5-C10-N21-C17
2	A	2095	3QH	C9-C10-N21-C17

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2095	3QH	5	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 than 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.



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, 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	847/966 (87%)	0.58	51 (6%) 27 24	15, 48, 77, 94	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	968	ILE	4.5
1	A	1084	PHE	4.0
1	A	915	SER	3.9
1	A	215	ILE	3.8
1	A	1042	LEU	3.8
1	A	216	ALA	3.8
1	A	749	ILE	3.7
1	A	969	LEU	3.7
1	A	287	ILE	3.5
1	A	779	LEU	3.3
1	A	1074	VAL	3.3
1	A	902	PHE	3.1
1	A	752	LEU	3.1
1	A	896	VAL	3.1
1	A	212	TRP	3.0
1	A	248	PHE	2.9
1	A	947	ARG	2.9
1	A	244	ILE	2.9
1	A	994	VAL	2.9
1	A	983	VAL	2.8
1	A	1088	LEU	2.8
1	A	892	GLN	2.8
1	A	1040	PRO	2.7
1	A	747	LEU	2.6
1	A	1083	GLN	2.6
1	A	910	TRP	2.5
1	A	966	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	489	GLY	2.4
1	A	233	ILE	2.4
1	A	898	ASN	2.4
1	A	375	ARG	2.4
1	A	917	THR	2.3
1	A	916	PRO	2.3
1	A	1072	ILE	2.3
1	A	374	PRO	2.3
1	A	765	SER	2.3
1	A	1041	GLN	2.2
1	A	245	LEU	2.2
1	A	1008	LYS	2.2
1	A	229	THR	2.2
1	A	929	VAL	2.1
1	A	1092	LEU	2.1
1	A	757	TYR	2.1
1	A	376	ASN	2.1
1	A	895	THR	2.1
1	A	987	LEU	2.1
1	A	272	LEU	2.1
1	A	1077	ASP	2.1
1	A	525	HIS	2.1
1	A	950	ASP	2.1
1	A	355	TRP	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](#)

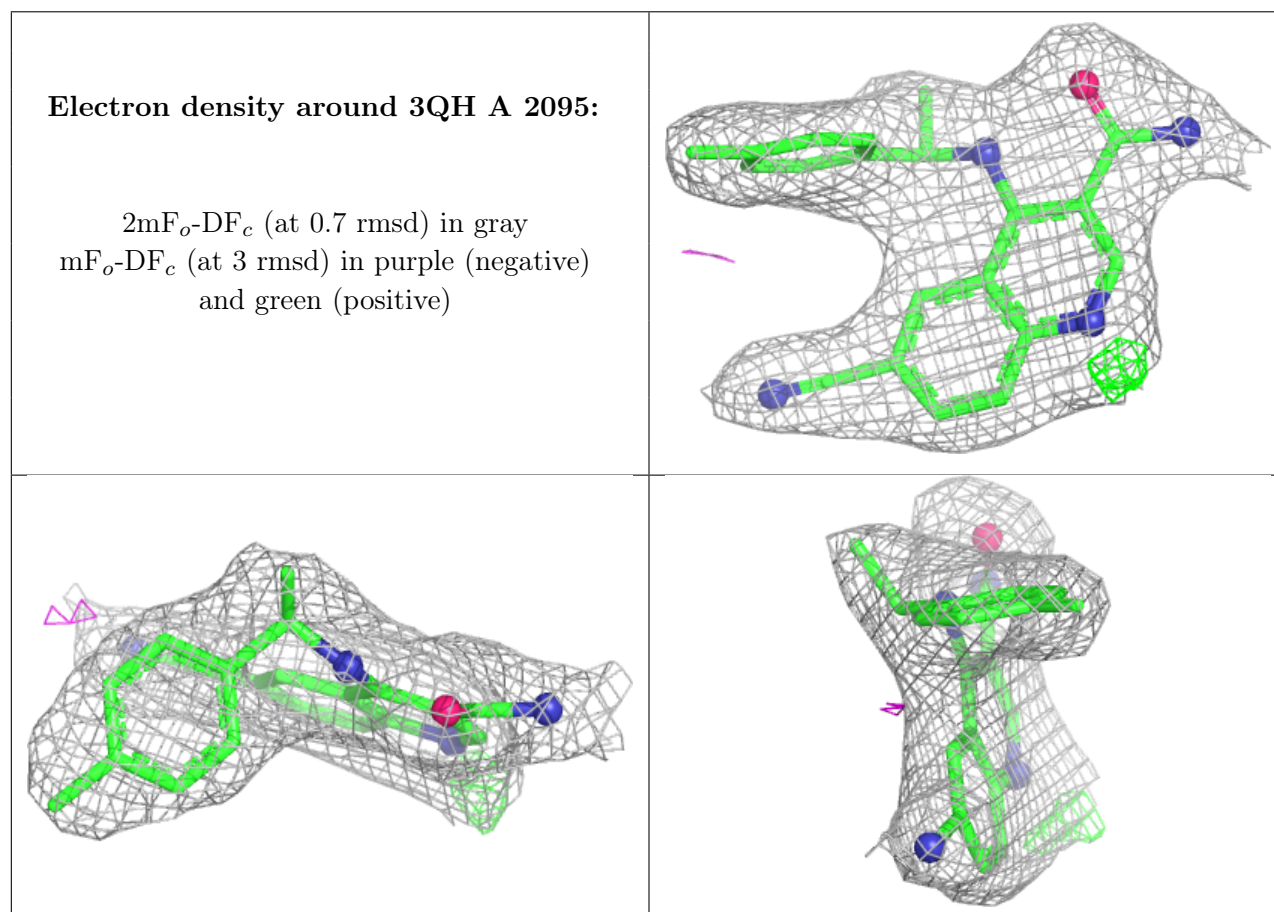
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	SO4	A	2096	5/5	0.78	0.10	79,79,80,81	0
2	3QH	A	2095	25/25	0.90	0.09	37,39,41,41	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.