



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:20 pm BST

PDB ID : 4AOF
Title : Selective small molecule inhibitor discovered by chemoproteomic assay platform reveals regulation of Th17 cell differentiation by PI3Kgamma
Authors : Bergamini, G.; Bell, K.; Shimamura, S.; Werner, T.; Cansfield, A.; Muller, K.; Perrin, J.; Rau, C.; Ellard, K.; Hopf, C.; Doce, C.; Leggate, D.; Mangano, R.; Mathieson, T.; OMahony, A.; Plavec, I.; Rharbaoui, F.; Reinhard, F.; Savitski, M.M.; Ramsden, N.; Hirsch, E.; Drewes, G.; Rausch, O.; Bantscheff, M.; Neubauer, G.
Deposited on : 2012-03-26
Resolution : 3.30 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 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	:	2.11
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)	:	2.11

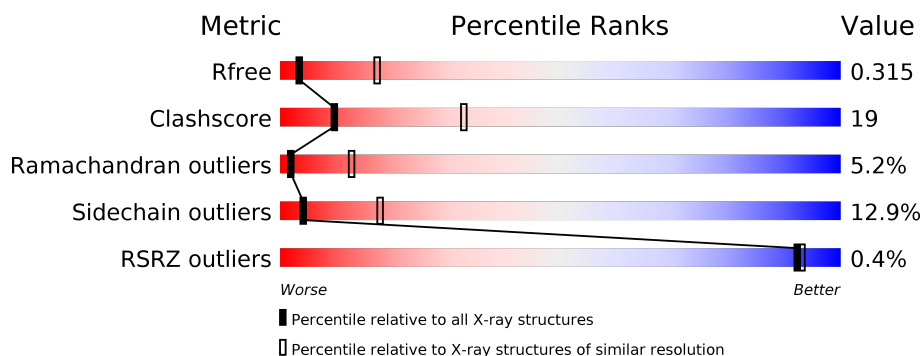
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	960	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6793 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.

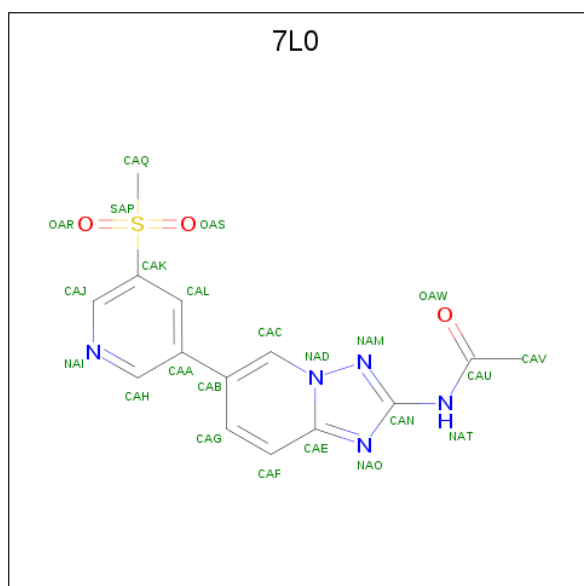
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	837	Total	C	N	O	S	0	0	1
			6741	4321	1152	1233	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736

- Molecule 2 is N-[6-(5-methylsulfonylpyridin-3-yl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl]ethanamide (three-letter code: 7L0) (formula: C₁₄H₁₃N₅O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	14	5	3	1		

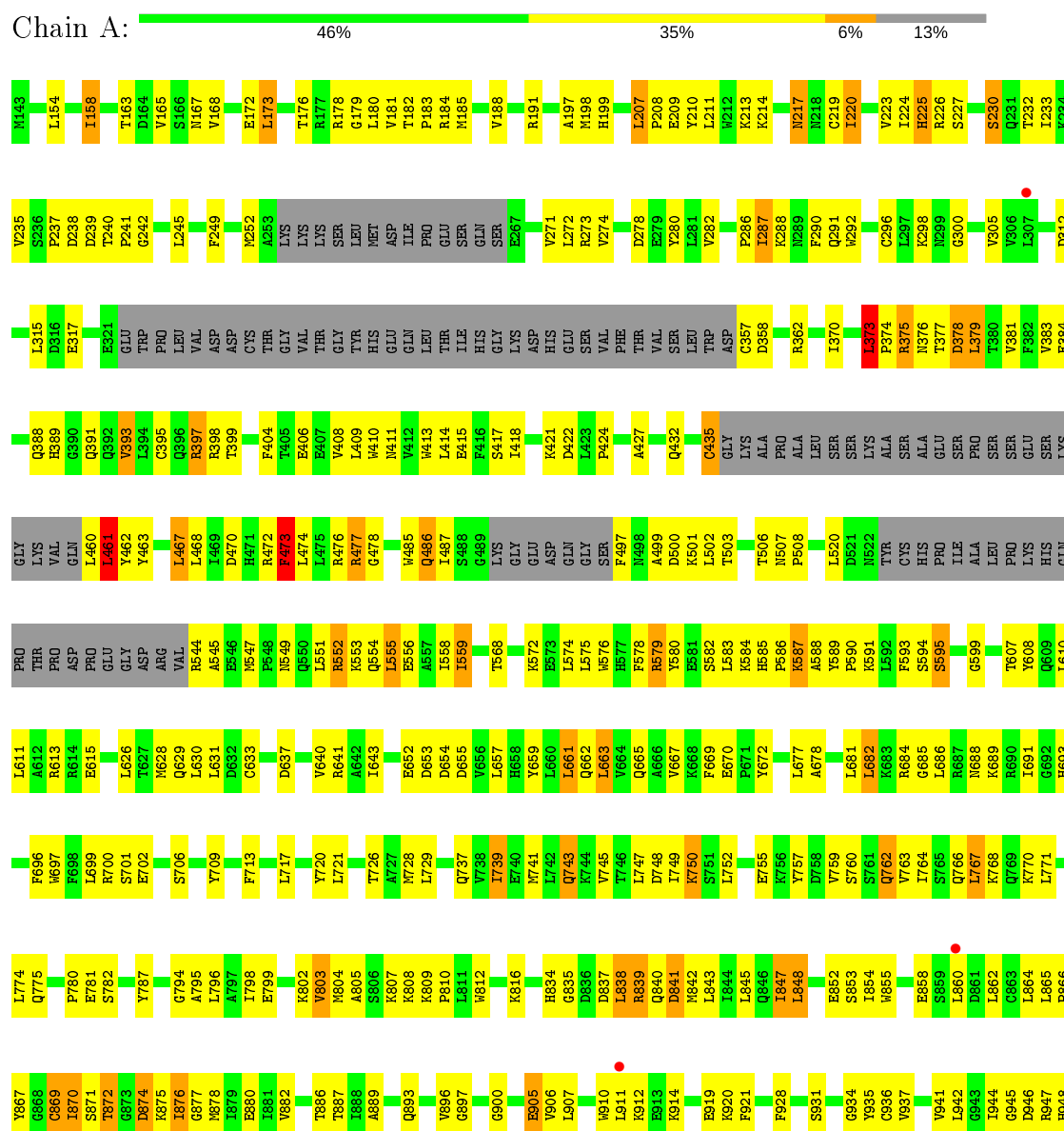
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



H949	D950	M953	E956	L960	F961	H962	I963	G966	H967	ILE	LEU	GLY	ASN	TYR	LYS	SER	PHE	LEU	GLY	ILE	ASN	LYS	GLU	ARG	V983	P984	F985	V986	P989	D990	F991	L992	F993	V994	T997	S998	G999	K1000	K1001	T1002	S1003	P1004	H1005	F1006	Q1007	K1008	F1009	Q1010	D1011	I1012	C1013	V1014
L1018	A1019	L1020	R1021	H1022	H1023	T1024	M1025	I1029	M1034	L1035	M1036	T1037	G1038	M1039	P1040	Q1041	L1042	T1043	S1044	K1045	E1046	D1047	I1048	E1049	Y1050	I1051	R1052	D1053	T1056	E1062	K1065	F1068	Q1071	I1072	R1076	D1077	K1078	Q1083	V1091	I1094	LYS	GLN	GLY	GLU	LYS	HIS	SER	ALA				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.77Å 68.05Å 109.87Å 90.00° 94.61° 90.00°	Depositor
Resolution (Å)	109.76 – 3.30 61.39 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (109.76-3.30) 93.7 (61.39-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.346 0.263 , 0.315	Depositor DCC
R_{free} test set	759 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	100.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6793	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7L0

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	0/6884	0.63	1/9316 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	767	LEU	CA-CB-CG	5.31	127.50	115.30

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	6741	0	6747	262	0
2	A	23	0	13	0	0
3	A	29	0	0	1	0
All	All	6793	0	6760	262	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 19.

All (262) 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:397:ARG:HH11	1:A:397:ARG:HG2	1.25	0.98
1:A:241:PRO:HG2	1:A:290:PHE:CE1	2.00	0.95
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.46	0.94
1:A:628:MET:HB3	1:A:1029:ILE:HD11	1.54	0.88
1:A:397:ARG:HH11	1:A:397:ARG:CG	1.88	0.86
1:A:864:LEU:O	1:A:866:PRO:HD3	1.76	0.84
1:A:576:TRP:O	1:A:579:ARG:HG3	1.79	0.82
1:A:375:ARG:HE	1:A:376:ASN:H	1.29	0.79
1:A:607:THR:HA	1:A:610:LEU:HD12	1.64	0.79
1:A:182:THR:HB	1:A:183:PRO:HD3	1.63	0.78
1:A:945:GLY:O	1:A:986:VAL:HG23	1.83	0.77
1:A:726:THR:HA	1:A:729:LEU:HB3	1.64	0.77
1:A:460:LEU:HG	1:A:461:LEU:H	1.47	0.77
1:A:874:ASP:O	1:A:876:ILE:N	2.19	0.76
1:A:1008:LYS:HG3	1:A:1012:ILE:HD11	1.68	0.75
1:A:375:ARG:NE	1:A:376:ASN:H	1.85	0.75
1:A:373:LEU:H	1:A:374:PRO:HD3	1.53	0.74
1:A:1000:LYS:HA	1:A:1076:ARG:HH11	1.50	0.74
1:A:241:PRO:HG2	1:A:290:PHE:HE1	1.50	0.72
1:A:460:LEU:HG	1:A:461:LEU:N	2.03	0.72
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.70	0.71
1:A:583:LEU:HD23	1:A:589:TYR:OH	1.92	0.70
1:A:397:ARG:HG2	1:A:397:ARG:NH1	1.96	0.70
1:A:743:GLN:HE21	1:A:876:ILE:HD12	1.57	0.69
1:A:497:PHE:N	1:A:1044:SER:HG	1.89	0.69
1:A:717:LEU:HD21	1:A:721:LEU:HD12	1.74	0.69
1:A:1039:MET:HB3	1:A:1040:PRO:CD	2.21	0.68
1:A:1000:LYS:HA	1:A:1076:ARG:NH1	2.09	0.68
1:A:287:ILE:HD12	1:A:288:LYS:H	1.59	0.67
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.75	0.67
1:A:240:THR:HG22	1:A:242:GLY:H	1.58	0.67
1:A:1043:THR:HG22	1:A:1045:LYS:H	1.61	0.66
1:A:182:THR:HB	1:A:183:PRO:CD	2.25	0.66
1:A:709:TYR:HB3	1:A:713:PHE:CD2	2.31	0.65
1:A:629:GLN:HG2	3:A:2016:HOH:O	1.95	0.65
1:A:158:ILE:HG23	1:A:717:LEU:HD22	1.78	0.65
1:A:750:LYS:HE3	1:A:809:LYS:H	1.62	0.65
1:A:1042:LEU:H	1:A:1042:LEU:HD13	1.60	0.65
1:A:1062:GLU:H	1:A:1062:GLU:CD	2.01	0.64
1:A:637:ASP:HB3	1:A:640:VAL:HG23	1.79	0.64
1:A:1043:THR:O	1:A:1048:ILE:HG12	1.97	0.64
1:A:808:LYS:O	1:A:810:PRO:HD3	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:MET:SD	1:A:663:LEU:HD23	2.38	0.64
1:A:181:VAL:HG13	1:A:184:ARG:HH21	1.64	0.63
1:A:178:ARG:C	1:A:180:LEU:H	2.01	0.62
1:A:889:ALA:HB2	1:A:950:ASP:HA	1.81	0.62
1:A:427:ALA:HB3	1:A:468:LEU:HB2	1.82	0.62
1:A:291:GLN:HG3	1:A:654:ASP:OD2	2.00	0.62
1:A:869:CYS:O	1:A:870:ILE:HD12	2.00	0.61
1:A:745:VAL:HG12	1:A:749:ILE:CD1	2.31	0.61
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.00	0.61
1:A:795:ALA:HB3	1:A:816:LYS:HD2	1.80	0.61
1:A:984:PRO:HG2	1:A:1071:GLN:OE1	2.00	0.61
1:A:587:LYS:HA	1:A:626:LEU:HD11	1.81	0.60
1:A:697:TRP:CZ3	1:A:872:THR:HG22	2.36	0.60
1:A:775:GLN:HG3	1:A:798:ILE:HD11	1.82	0.60
1:A:661:LEU:HG	1:A:843:LEU:HD13	1.84	0.60
1:A:185:MET:HA	1:A:188:VAL:HB	1.84	0.60
1:A:928:PHE:HZ	1:A:991:PHE:HD2	1.50	0.59
1:A:886:THR:HG22	1:A:887:THR:H	1.65	0.59
1:A:990:ASP:O	1:A:994:VAL:HG23	2.01	0.59
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.85	0.59
1:A:787:TYR:HB3	1:A:870:ILE:CD1	2.33	0.59
1:A:1000:LYS:HG2	1:A:1076:ARG:HD2	1.83	0.58
1:A:547:MET:HB3	1:A:578:PHE:CE1	2.39	0.58
1:A:273:ARG:O	1:A:305:VAL:HG13	2.03	0.58
1:A:709:TYR:HB3	1:A:713:PHE:HD2	1.68	0.58
1:A:631:LEU:O	1:A:641:ARG:NH2	2.36	0.57
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.40	0.57
1:A:397:ARG:NH1	1:A:397:ARG:CG	2.58	0.57
1:A:271:VAL:HG21	1:A:282:VAL:HG22	1.86	0.57
1:A:211:LEU:HA	1:A:214:LYS:HB3	1.87	0.57
1:A:389:HIS:CD2	1:A:424:PRO:HB2	2.39	0.57
1:A:787:TYR:HB3	1:A:870:ILE:HD13	1.87	0.57
1:A:867:TYR:HB2	1:A:880:GLU:HB3	1.85	0.57
1:A:1039:MET:HB2	1:A:1042:LEU:HD12	1.86	0.56
1:A:373:LEU:HD23	1:A:374:PRO:HD3	1.87	0.56
1:A:802:LYS:HG3	1:A:812:TRP:HB3	1.87	0.56
1:A:460:LEU:CG	1:A:461:LEU:H	2.17	0.56
1:A:245:LEU:HD23	1:A:249:PHE:CE1	2.41	0.56
1:A:887:THR:HG22	1:A:889:ALA:H	1.70	0.56
1:A:154:LEU:O	1:A:158:ILE:HG13	2.06	0.55
1:A:315:LEU:C	1:A:317:GLU:H	2.09	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ILE:HD13	1:A:872:THR:HB	1.88	0.55
1:A:997:THR:HG23	1:A:1001:LYS:H	1.70	0.55
1:A:1034:MET:HE3	1:A:1039:MET:HE3	1.89	0.55
1:A:937:VAL:O	1:A:941:VAL:HG23	2.07	0.55
1:A:760:SER:O	1:A:763:VAL:HG12	2.07	0.55
1:A:589:TYR:O	1:A:593:PHE:HD2	1.91	0.54
1:A:842:MET:HE1	1:A:871:SER:H	1.72	0.54
1:A:176:THR:O	1:A:180:LEU:HG	2.08	0.54
1:A:178:ARG:O	1:A:180:LEU:N	2.40	0.54
1:A:889:ALA:O	1:A:893:GLN:HG3	2.08	0.54
1:A:357:CYS:SG	1:A:358:ASP:N	2.80	0.54
1:A:467:LEU:O	1:A:476:ARG:NH1	2.41	0.54
1:A:747:LEU:HA	1:A:750:LYS:HB2	1.90	0.54
1:A:745:VAL:HG12	1:A:749:ILE:HD13	1.90	0.54
1:A:395:CYS:SG	1:A:417:SER:OG	2.66	0.53
1:A:1025:ASN:O	1:A:1029:ILE:HG22	2.08	0.53
1:A:947:ARG:HH21	1:A:962:HIS:HB3	1.74	0.53
1:A:852:GLU:HG2	1:A:855:TRP:HE3	1.73	0.53
1:A:910:TRP:CH2	1:A:956:GLU:HG3	2.44	0.52
1:A:373:LEU:H	1:A:374:PRO:CD	2.22	0.52
1:A:934:GLY:C	1:A:936:CYS:H	2.12	0.52
1:A:628:MET:HB3	1:A:1029:ILE:CD1	2.33	0.52
1:A:928:PHE:HZ	1:A:991:PHE:CD2	2.26	0.52
1:A:1039:MET:CB	1:A:1040:PRO:HD2	2.29	0.52
1:A:241:PRO:CG	1:A:290:PHE:CE1	2.86	0.52
1:A:296:CYS:O	1:A:300:GLY:N	2.43	0.52
1:A:373:LEU:N	1:A:374:PRO:HD3	2.24	0.52
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.91	0.52
1:A:1043:THR:HB	1:A:1046:GLU:HB2	1.91	0.52
1:A:841:ASP:O	1:A:845:LEU:HD22	2.10	0.52
1:A:946:ASP:HB2	1:A:983:VAL:HG12	1.90	0.51
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.40	0.51
1:A:499:ALA:C	1:A:501:LYS:H	2.14	0.51
1:A:580:TYR:HA	1:A:583:LEU:HD12	1.91	0.51
1:A:287:ILE:CD1	1:A:288:LYS:H	2.22	0.51
1:A:684:ARG:HA	1:A:684:ARG:NE	2.25	0.51
1:A:886:THR:HG22	1:A:887:THR:N	2.26	0.51
1:A:1018:LEU:HA	1:A:1021:ARG:HB2	1.92	0.51
1:A:373:LEU:N	1:A:374:PRO:CD	2.74	0.51
1:A:641:ARG:HE	1:A:670:GLU:HG2	1.76	0.50
1:A:847:ILE:HG21	1:A:942:LEU:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:THR:HG23	1:A:1006:PHE:HD2	1.76	0.50
1:A:271:VAL:HG22	1:A:272:LEU:N	2.27	0.50
1:A:780:PRO:O	1:A:782:SER:N	2.45	0.50
1:A:928:PHE:CZ	1:A:991:PHE:HD2	2.28	0.49
1:A:549:ASN:O	1:A:552:ARG:HG2	2.12	0.49
1:A:1018:LEU:HD13	1:A:1022:HIS:HE1	1.77	0.49
1:A:737:GLN:O	1:A:741:MET:HG2	2.12	0.49
1:A:678:ALA:HA	1:A:681:LEU:HD12	1.94	0.49
1:A:211:LEU:HD11	1:A:298:LYS:HA	1.95	0.49
1:A:585:HIS:HB3	1:A:587:LYS:NZ	2.27	0.49
1:A:667:VAL:C	1:A:669:PHE:H	2.16	0.49
1:A:787:TYR:CA	1:A:870:ILE:HD13	2.43	0.48
1:A:1068:PHE:O	1:A:1072:ILE:HG13	2.13	0.48
1:A:178:ARG:C	1:A:180:LEU:N	2.67	0.48
1:A:589:TYR:O	1:A:593:PHE:CD2	2.65	0.48
1:A:689:LYS:HE3	1:A:728:MET:HG2	1.95	0.48
1:A:842:MET:CE	1:A:871:SER:H	2.26	0.48
1:A:654:ASP:HA	1:A:657:LEU:HD12	1.95	0.48
1:A:558:ILE:HG21	1:A:575:LEU:HD11	1.96	0.48
1:A:862:LEU:O	1:A:931:SER:HA	2.14	0.48
1:A:223:VAL:HG22	1:A:232:THR:HG23	1.94	0.48
1:A:702:GLU:OE1	1:A:839:ARG:NH1	2.47	0.48
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.96	0.48
1:A:556:GLU:HA	1:A:559:ILE:HB	1.96	0.48
1:A:172:GLU:OE2	1:A:672:TYR:HD1	1.97	0.48
1:A:191:ARG:HD3	1:A:686:LEU:O	2.14	0.48
1:A:699:LEU:HD23	1:A:713:PHE:HD1	1.79	0.48
1:A:739:ILE:HG21	1:A:872:THR:HG21	1.96	0.48
1:A:271:VAL:HG22	1:A:272:LEU:H	1.77	0.47
1:A:887:THR:HA	1:A:953:MET:HG2	1.95	0.47
1:A:990:ASP:OD1	1:A:990:ASP:N	2.47	0.47
1:A:207:LEU:HD11	1:A:288:LYS:HB2	1.95	0.47
1:A:224:ILE:O	1:A:230:SER:HA	2.15	0.47
1:A:485:TRP:CH2	1:A:508:PRO:HD3	2.49	0.47
1:A:579:ARG:HB3	1:A:610:LEU:HD21	1.97	0.47
1:A:427:ALA:HB1	1:A:468:LEU:HD12	1.96	0.47
1:A:1044:SER:HA	1:A:1048:ILE:HG13	1.96	0.47
1:A:749:ILE:HG21	1:A:803:VAL:HG11	1.96	0.47
1:A:802:LYS:CG	1:A:812:TRP:HB3	2.45	0.47
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.96	0.47
1:A:211:LEU:HD21	1:A:298:LYS:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:HG12	1:A:409:LEU:N	2.30	0.47
1:A:782:SER:HA	1:A:794:GLY:HA2	1.96	0.47
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.15	0.47
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.97	0.47
1:A:220:ILE:HD12	1:A:235:VAL:HG12	1.96	0.47
1:A:787:TYR:HA	1:A:870:ILE:CD1	2.45	0.47
1:A:854:ILE:HG21	1:A:1020:LEU:HD23	1.97	0.46
1:A:1056:THR:HG23	1:A:1056:THR:O	2.15	0.46
1:A:766:GLN:O	1:A:770:LYS:HD3	2.16	0.46
1:A:379:LEU:HD12	1:A:435:CYS:SG	2.56	0.46
1:A:726:THR:HA	1:A:729:LEU:CB	2.42	0.46
1:A:764:ILE:HG12	1:A:803:VAL:HG23	1.97	0.46
1:A:544:ARG:HB3	1:A:544:ARG:NH1	2.31	0.45
1:A:752:LEU:HD13	1:A:762:GLN:HE21	1.81	0.45
1:A:1050:TYR:C	1:A:1050:TYR:CD1	2.90	0.45
1:A:768:LYS:HA	1:A:771:LEU:HD12	1.98	0.45
1:A:696:PHE:CZ	1:A:700:ARG:HD2	2.51	0.45
1:A:485:TRP:CZ3	1:A:507:ASN:HA	2.52	0.45
1:A:432:GLN:HE21	1:A:460:LEU:HD11	1.82	0.45
1:A:239:ASP:O	1:A:287:ILE:HG13	2.16	0.45
1:A:590:PRO:O	1:A:594:SER:OG	2.32	0.45
1:A:486:GLN:HG3	1:A:487:ILE:N	2.31	0.45
1:A:729:LEU:O	1:A:729:LEU:HD23	2.17	0.45
1:A:1043:THR:C	1:A:1045:LYS:H	2.21	0.44
1:A:591:LYS:O	1:A:595:SER:OG	2.33	0.44
1:A:709:TYR:HB3	1:A:713:PHE:CE2	2.52	0.44
1:A:273:ARG:HG3	1:A:280:TYR:CE1	2.52	0.44
1:A:693:HIS:O	1:A:696:PHE:HB3	2.18	0.44
1:A:684:ARG:HE	1:A:684:ARG:HA	1.82	0.44
1:A:741:MET:HB3	1:A:774:LEU:HD13	2.00	0.44
1:A:1018:LEU:HD13	1:A:1022:HIS:CE1	2.52	0.44
1:A:198:MET:O	1:A:280:TYR:HB2	2.18	0.44
1:A:470:ASP:OD2	1:A:472:ARG:HD2	2.17	0.44
1:A:586:PRO:C	1:A:588:ALA:H	2.21	0.44
1:A:686:LEU:HD23	1:A:720:TYR:HE1	1.82	0.44
1:A:391:GLN:NE2	1:A:502:LEU:HD11	2.33	0.44
1:A:235:VAL:HG13	1:A:239:ASP:HB2	2.00	0.43
1:A:383:VAL:HG12	1:A:384:GLU:N	2.32	0.43
1:A:665:GLN:HB3	1:A:1037:THR:HG21	2.00	0.43
1:A:834:HIS:CG	1:A:835:GLY:N	2.85	0.43
1:A:461:LEU:HD22	1:A:462:TYR:CD2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ARG:HH21	1:A:478:GLY:HA2	1.83	0.43
1:A:207:LEU:HA	1:A:208:PRO:HD2	1.77	0.43
1:A:640:VAL:O	1:A:643:ILE:HG12	2.18	0.43
1:A:631:LEU:HD13	1:A:677:LEU:HD22	2.01	0.43
1:A:197:ALA:HA	1:A:689:LYS:NZ	2.34	0.43
1:A:373:LEU:HD22	1:A:406:GLU:HG2	2.01	0.43
1:A:399:THR:HG22	1:A:414:LEU:HD21	2.00	0.43
1:A:655:ASP:O	1:A:659:TYR:CD2	2.72	0.43
1:A:167:ASN:HD21	1:A:506:THR:H	1.66	0.43
1:A:685:GLY:HA2	1:A:691:ILE:CG2	2.46	0.42
1:A:865:LEU:HD21	1:A:882:VAL:HG11	2.02	0.42
1:A:919:GLU:O	1:A:921:PHE:N	2.51	0.42
1:A:907:LEU:HD22	1:A:994:VAL:HG21	2.00	0.42
1:A:1034:MET:HE2	1:A:1039:MET:HE2	2.02	0.42
1:A:393:VAL:O	1:A:393:VAL:HG23	2.20	0.42
1:A:701:SER:HB2	1:A:871:SER:HB3	2.02	0.42
1:A:905:GLU:HG3	1:A:905:GLU:H	1.68	0.42
1:A:655:ASP:O	1:A:659:TYR:HD2	2.02	0.42
1:A:315:LEU:C	1:A:317:GLU:N	2.73	0.42
1:A:472:ARG:O	1:A:473:PHE:HB2	2.20	0.42
1:A:226:ARG:HB3	1:A:227:SER:H	1.75	0.42
1:A:427:ALA:CB	1:A:468:LEU:HB2	2.49	0.42
1:A:499:ALA:HB2	1:A:1036:MET:HB3	2.02	0.42
1:A:165:VAL:HB	1:A:168:VAL:HG21	2.02	0.42
1:A:477:ARG:NH2	1:A:478:GLY:HA2	2.34	0.42
1:A:667:VAL:C	1:A:669:PHE:N	2.73	0.42
1:A:225:HIS:N	1:A:225:HIS:ND1	2.68	0.41
1:A:553:LYS:C	1:A:555:LEU:H	2.24	0.41
1:A:689:LYS:CE	1:A:728:MET:HG2	2.50	0.41
1:A:914:LYS:HD3	1:A:914:LYS:HA	1.78	0.41
1:A:682:LEU:HD21	1:A:720:TYR:HA	2.01	0.41
1:A:210:TYR:CD1	1:A:211:LEU:HG	2.54	0.41
1:A:608:TYR:HA	1:A:611:LEU:HD12	2.03	0.41
1:A:838:LEU:HD22	1:A:838:LEU:N	2.35	0.41
1:A:1021:ARG:O	1:A:1023:HIS:N	2.53	0.41
1:A:944:ILE:O	1:A:947:ARG:HD3	2.21	0.41
1:A:630:LEU:HA	1:A:630:LEU:HD23	1.82	0.41
1:A:209:GLU:O	1:A:213:LYS:HB3	2.21	0.41
1:A:224:ILE:HD13	1:A:233:ILE:HD13	2.03	0.41
1:A:771:LEU:CD1	1:A:798:ILE:HG23	2.51	0.41
1:A:413:TRP:O	1:A:414:LEU:HD23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASP:HB3	1:A:599:GLY:O	2.21	0.41
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	2.03	0.40
1:A:787:TYR:HA	1:A:870:ILE:HD11	2.02	0.40
1:A:210:TYR:O	1:A:214:LYS:HB2	2.21	0.40
1:A:477:ARG:HG2	1:A:520:LEU:O	2.20	0.40
1:A:544:ARG:HB3	1:A:544:ARG:CZ	2.51	0.40
1:A:551:LEU:HD22	1:A:574:LEU:HD21	2.02	0.40
1:A:1010:GLN:HG3	1:A:1010:GLN:H	1.75	0.40
1:A:198:MET:O	1:A:199:HIS:C	2.59	0.40
1:A:217:ASN:HD22	1:A:219:CYS:H	1.68	0.40
1:A:312:ASP:HB3	1:A:315:LEU:HD12	2.03	0.40
1:A:947:ARG:O	1:A:948:HIS:C	2.60	0.40
1:A:576:TRP:O	1:A:579:ARG:NE	2.54	0.40
1:A:629:GLN:HA	1:A:1029:ILE:HG13	2.02	0.40
1:A:914:LYS:HG3	1:A:956:GLU:HG2	2.02	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	823/960 (86%)	638 (78%)	142 (17%)	43 (5%)	2 13

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	PHE
1	A	579	ARG
1	A	615	GLU
1	A	755	GLU
1	A	781	GLU
1	A	874	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	875	LYS
1	A	897	GLY
1	A	1023	HIS
1	A	1040	PRO
1	A	173	LEU
1	A	179	GLY
1	A	378	ASP
1	A	393	VAL
1	A	461	LEU
1	A	500	ASP
1	A	584	LYS
1	A	762	GLN
1	A	900	GLY
1	A	949	ASN
1	A	963	ILE
1	A	1044	SER
1	A	286	PRO
1	A	572	LYS
1	A	653	ASP
1	A	757	TYR
1	A	805	ALA
1	A	839	ARG
1	A	847	ILE
1	A	920	LYS
1	A	1046	GLU
1	A	545	ALA
1	A	554	GLN
1	A	1050	TYR
1	A	238	ASP
1	A	848	LEU
1	A	906	VAL
1	A	935	TYR
1	A	966	GLY
1	A	1091	VAL
1	A	373	LEU
1	A	989	PRO
1	A	999	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	742/858 (86%)	646 (87%)	96 (13%)	4 18

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ILE
1	A	163	THR
1	A	173	LEU
1	A	207	LEU
1	A	217	ASN
1	A	220	ILE
1	A	225	HIS
1	A	230	SER
1	A	252	MET
1	A	278	ASP
1	A	287	ILE
1	A	362	ARG
1	A	370	ILE
1	A	373	LEU
1	A	375	ARG
1	A	377	THR
1	A	378	ASP
1	A	379	LEU
1	A	381	VAL
1	A	388	GLN
1	A	397	ARG
1	A	398	ARG
1	A	404	PHE
1	A	410	TRP
1	A	411	ASN
1	A	415	GLU
1	A	418	ILE
1	A	421	LYS
1	A	435	CYS
1	A	461	LEU
1	A	463	TYR
1	A	467	LEU
1	A	473	PHE
1	A	474	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	477	ARG
1	A	486	GLN
1	A	503	THR
1	A	552	ARG
1	A	555	LEU
1	A	559	ILE
1	A	568	THR
1	A	582	SER
1	A	587	LYS
1	A	595	SER
1	A	613	ARG
1	A	633	CYS
1	A	652	GLU
1	A	661	LEU
1	A	662	GLN
1	A	663	LEU
1	A	682	LEU
1	A	688	ASN
1	A	706	SER
1	A	739	ILE
1	A	743	GLN
1	A	748	ASP
1	A	750	LYS
1	A	759	VAL
1	A	767	LEU
1	A	796	LEU
1	A	799	GLU
1	A	803	VAL
1	A	804	MET
1	A	807	LYS
1	A	837	ASP
1	A	838	LEU
1	A	840	GLN
1	A	841	ASP
1	A	848	LEU
1	A	853	SER
1	A	858	GLU
1	A	860	LEU
1	A	869	CYS
1	A	870	ILE
1	A	872	THR
1	A	876	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	878	MET
1	A	896	VAL
1	A	905	GLU
1	A	911	LEU
1	A	912	LYS
1	A	949	ASN
1	A	960	LEU
1	A	1002	THR
1	A	1003	SER
1	A	1023	HIS
1	A	1029	ILE
1	A	1035	LEU
1	A	1037	THR
1	A	1042	LEU
1	A	1049	GLU
1	A	1052	ARG
1	A	1053	ASP
1	A	1076	ARG
1	A	1078	LYS
1	A	1083	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	217	ASN
1	A	268	GLN
1	A	304	HIS
1	A	391	GLN
1	A	432	GLN
1	A	710	GLN
1	A	743	GLN
1	A	762	GLN
1	A	766	GLN
1	A	769	GLN
1	A	846	GLN
1	A	893	GLN
1	A	948	HIS
1	A	951	ASN
1	A	1007	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 carbohydrates 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	7L0	A	2095	-	21,25,25	1.43	4 (19%)	25,37,37	2.21	8 (32%)

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	7L0	A	2095	-	-	4/12/14/14	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	7L0	CAA-CAB	-3.60	1.40	1.49
2	A	2095	7L0	OAR-SAP	2.52	1.51	1.44
2	A	2095	7L0	CAN-NAT	-2.50	1.35	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	7L0	OAS-SAP	2.39	1.50	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2095	7L0	OAR-SAP-OAS	-6.28	107.11	117.92
2	A	2095	7L0	CAQ-SAP-CAK	4.14	109.47	104.58
2	A	2095	7L0	CAL-CAK-SAP	3.73	122.02	119.06
2	A	2095	7L0	CAN-NAT-CAU	-2.91	125.88	130.28
2	A	2095	7L0	OAS-SAP-CAK	2.80	110.53	108.25
2	A	2095	7L0	CAJ-NAI-CAH	2.76	121.25	117.48
2	A	2095	7L0	OAR-SAP-CAK	2.35	110.16	108.25
2	A	2095	7L0	CAA-CAL-CAK	-2.24	118.18	119.96

There are no chirality outliers.

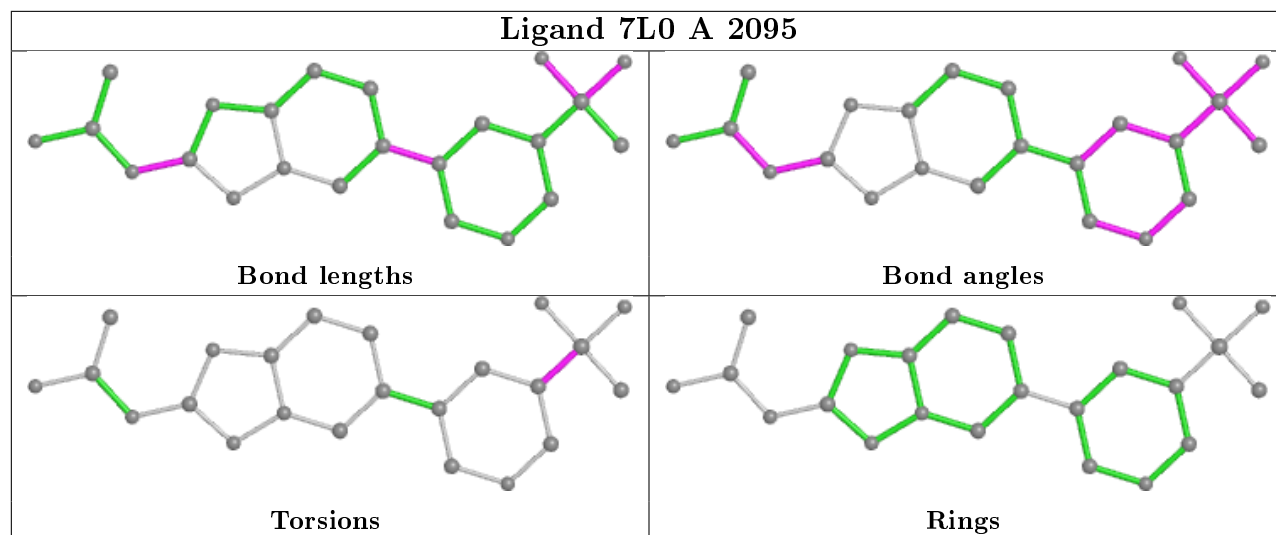
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2095	7L0	CAJ-CAK-SAP-OAR
2	A	2095	7L0	CAL-CAK-SAP-OAR
2	A	2095	7L0	CAL-CAK-SAP-CAQ
2	A	2095	7L0	CAJ-CAK-SAP-CAQ

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	837/960 (87%)	-0.04	3 (0%) 92 93	47, 66, 79, 90	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	3.6
1	A	860	LEU	2.8
1	A	911	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

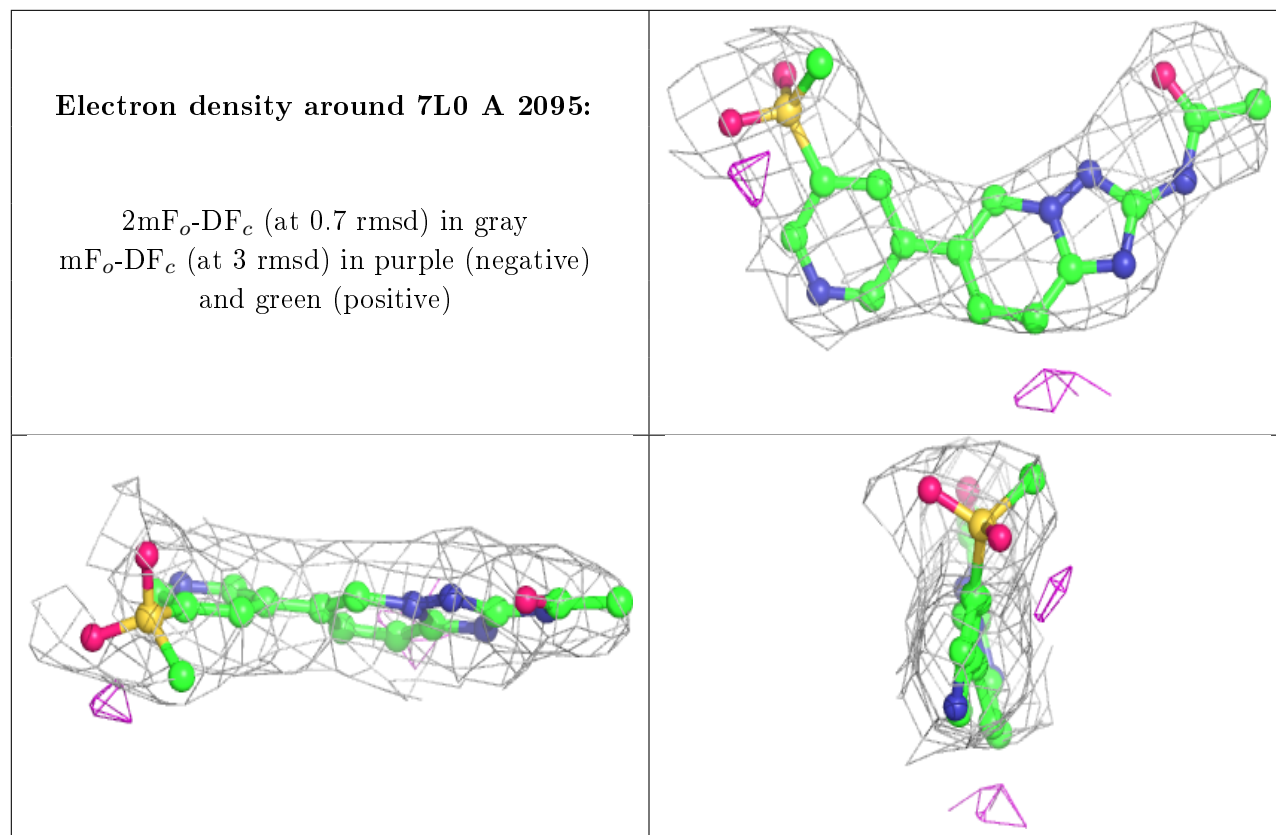
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	7L0	A	2095	23/23	0.93	0.22	55,57,59,59	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.