



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:15 AM EDT

PDB ID : 4AOF / pdb_00004aof
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 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

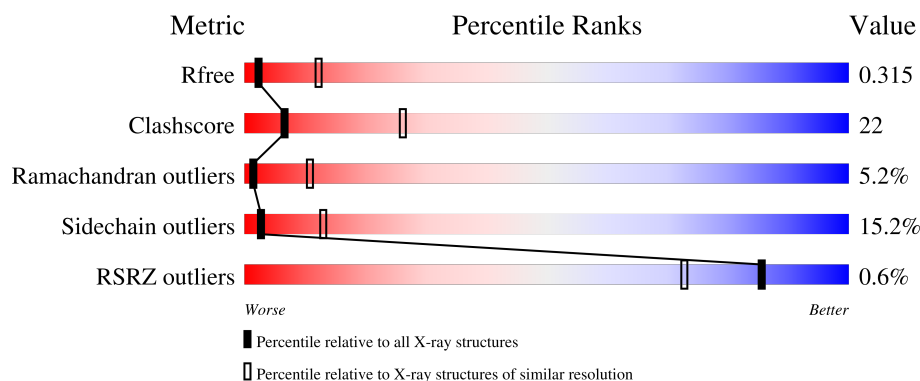
1 Overall quality at a glance

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	960	

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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.

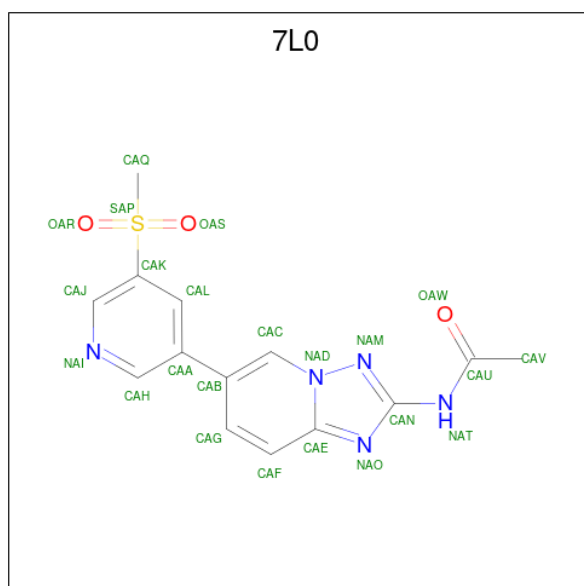
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

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

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 (CCD ID: 7L0) (formula: C₁₄H₁₃N₅O₃S).



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

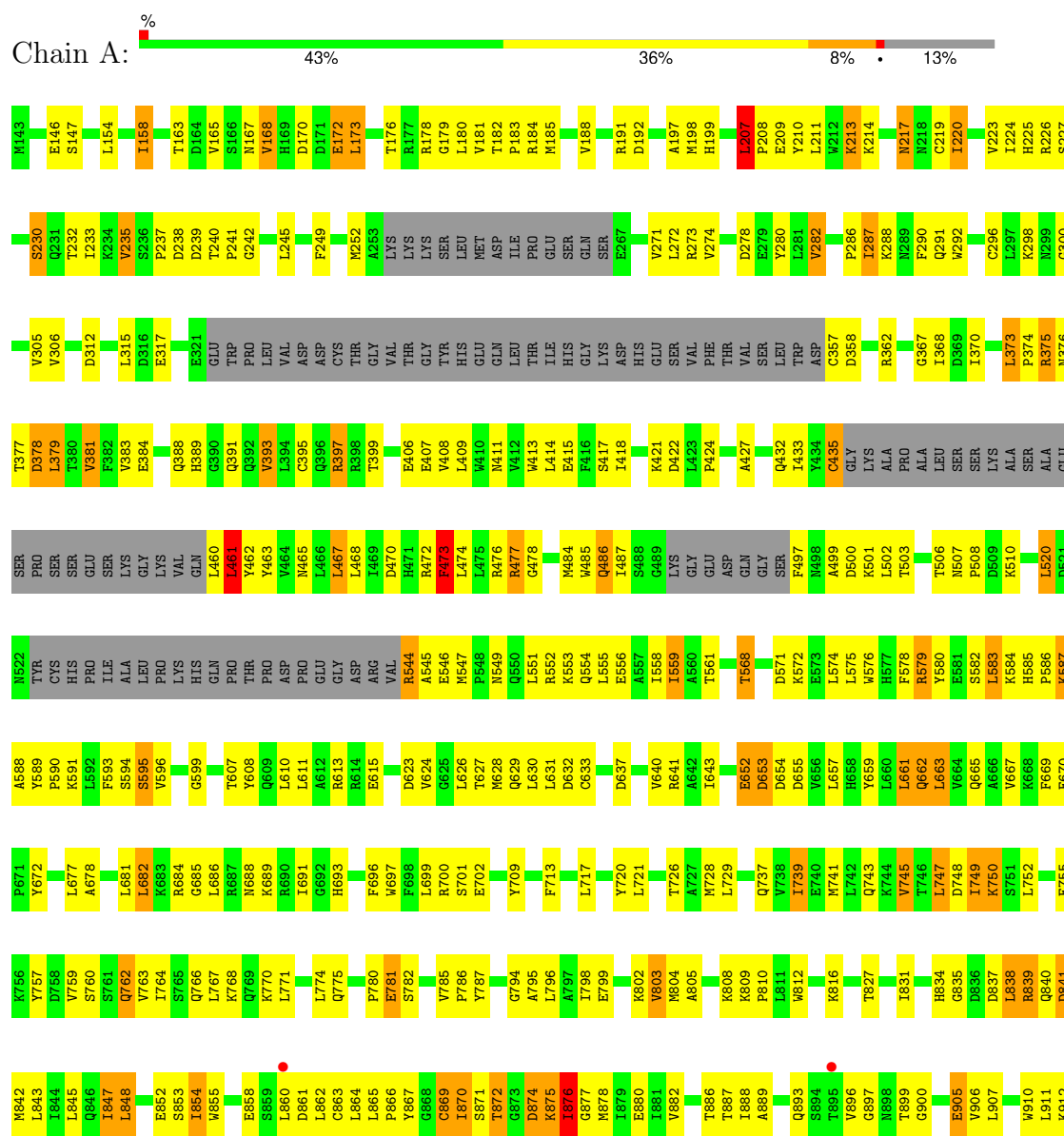
- Molecule 3 is water.

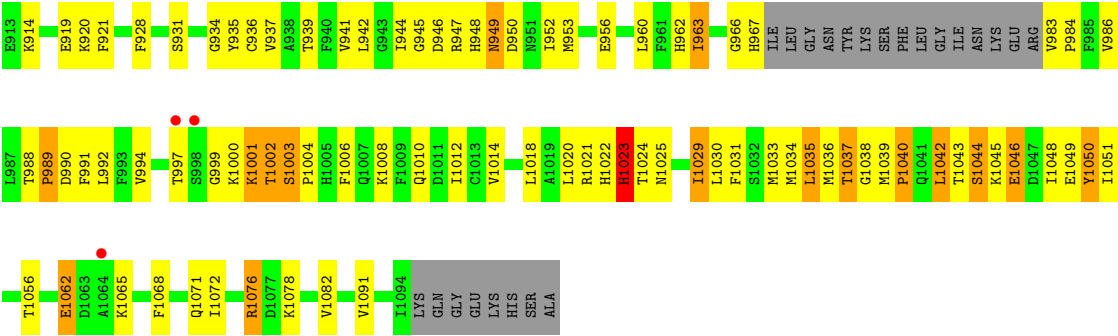
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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





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 – 3.30 109.52 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (109.76-3.30) 93.7 (109.52-3.30)	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 0.262 , 0.315	Depositor DCC
R_{free} test set	759 reflections (4.79%)	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 , 76.5	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	0.60	2/6884 (0.0%)	0.92	10/9316 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	C-O	6.12	1.30	1.23
1	A	876	ILE	CA-CB	5.84	1.62	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	VAL	N-CA-C	6.44	116.30	108.06
1	A	899	THR	N-CA-C	-5.73	107.28	114.56
1	A	207	LEU	CA-C-N	5.60	126.84	119.84
1	A	207	LEU	C-N-CA	5.60	126.84	119.84
1	A	988	THR	CA-C-N	5.44	126.64	119.84
1	A	988	THR	C-N-CA	5.44	126.64	119.84
1	A	170	ASP	N-CA-C	5.41	114.98	107.73
1	A	367	GLY	N-CA-C	5.09	117.06	110.45
1	A	465	ASN	N-CA-C	5.05	117.35	109.52
1	A	172	GLU	N-CA-C	-5.04	105.86	111.36

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	292	0
2	A	23	0	13	1	0
3	A	29	0	0	1	0
All	All	6793	0	6760	292	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 22.

All (292) 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:1034:MET:HE3	1:A:1039:MET:HE3	1.30	1.11
1:A:397:ARG:HG2	1:A:397:ARG:HH11	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:628:MET:HE1	1:A:662:GLN:HB3	1.58	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:1034:MET:CE	1:A:1039:MET:HE3	2.09	0.78
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:632:ASP:HA	1:A:1033:MET:HE3	1.72	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:LEU:HD21	1:A:721:LEU:HD12	1.74	0.69
1:A:1062:GLU:CD	1:A:1062:GLU:H	2.01	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:178:ARG:C	1:A:180:LEU:H	2.01	0.67
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:1034:MET:HE3	1:A:1039:MET:CE	2.18	0.66
1:A:831:ILE:HG21	2:A:2095:7L0:HAQ3	1.76	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:158:ILE:HG23	1:A:717:LEU:HD22	1.78	0.65
1:A:629:GLN:HG2	3:A:2016:HOH:O	1.95	0.65
1:A:750:LYS:HE3	1:A:809:LYS:H	1.62	0.65
1:A:1042:LEU:HD13	1:A:1042:LEU:H	1.60	0.65
1:A:637:ASP:HB3	1:A:640:VAL:HG23	1.79	0.64
1:A:497:PHE:N	1:A:1044:SER:HG	1.96	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
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:889:ALA:HB2	1:A:950:ASP:HA	1.81	0.62
1:A:1038:GLY:HA3	1:A:1039:MET:HE2	1.80	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:315:LEU:C	1:A:317:GLU:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:842:MET:HE2	1:A:871:SER:H	1.67	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:842:MET:HE2	1:A:871:SER:N	2.19	0.58
1:A:934:GLY:C	1:A:936:CYS:H	2.12	0.57
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:CG	1:A:397:ARG:NH1	2.58	0.57
1:A:395:CYS:HG	1:A:417:SER:HG	1.52	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: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: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:499:ALA:C	1:A:501:LYS:H	2.14	0.54
1:A:667:VAL:C	1:A:669:PHE:H	2.16	0.54
1:A:589:TYR:O	1:A:593:PHE:HD2	1.91	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:576:TRP:NE1	1:A:579:ARG:HH21	2.07	0.53
1:A:1025:ASN:O	1:A:1029:ILE:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:C	1:A:180:LEU:N	2.67	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: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: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:1039:MET:CB	1:A:1040:PRO:HD2	2.29	0.52
1:A:841:ASP:O	1:A:845:LEU:HD22	2.10	0.52
1:A:1043:THR:HB	1:A:1046:GLU:HB2	1.91	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: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:373:LEU:N	1:A:374:PRO:CD	2.74	0.51
1:A:1018:LEU:HA	1:A:1021:ARG:HB2	1.92	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
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:1050:TYR:CD1	1:A:1050:TYR:C	2.90	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:737:GLN:O	1:A:741:MET:HG2	2.12	0.49
1:A:1018:LEU:HD13	1:A:1022:HIS:HE1	1.77	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:787:TYR:CA	1:A:870:ILE:HD13	2.43	0.48
1:A:586:PRO:C	1:A:588:ALA:H	2.21	0.48
1:A:1068:PHE:O	1:A:1072:ILE:HG13	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1043:THR:C	1:A:1045:LYS:H	2.21	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: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: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:433:ILE:HG13	1:A:484:MET:HE1	1.97	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:315:LEU:C	1:A:317:GLU:N	2.73	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: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:1044:SER:HA	1:A:1048:ILE:HG13	1.96	0.47
1:A:211:LEU:HD21	1:A:298:LYS:HA	1.97	0.47
1:A:408:VAL:HG12	1:A:409:LEU:N	2.30	0.47
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.96	0.47
1:A:782:SER:HA	1:A:794:GLY:HA2	1.96	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: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: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:553:LYS:C	1:A:555:LEU:H	2.24	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:591:LYS:O	1:A:595:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ARG:NH1	1:A:544:ARG:HB3	2.31	0.45
1:A:752:LEU:HD13	1:A:762:GLN:HE21	1.81	0.45
1:A:768:LYS:HA	1:A:771:LEU:HD12	1.98	0.45
1:A:198:MET:O	1:A:199:HIS:C	2.59	0.45
1:A:696:PHE:CZ	1:A:700:ARG:HD2	2.51	0.45
1:A:947:ARG:O	1:A:948:HIS:C	2.60	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:1030:LEU:O	1:A:1031:PHE:C	2.59	0.45
1:A:486:GLN:HG3	1:A:487:ILE:N	2.31	0.45
1:A:729:LEU:HD23	1:A:729:LEU:O	2.17	0.45
1:A:869:CYS:C	1:A:870:ILE:HD12	2.42	0.45
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:HA	1:A:684:ARG:HE	1.82	0.44
1:A:741:MET:HB3	1:A:774:LEU:HD13	2.00	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:686:LEU:HD23	1:A:720:TYR:HE1	1.82	0.44
1:A:1018:LEU:HD13	1:A:1022:HIS:CE1	2.52	0.44
1:A:391:GLN:NE2	1:A:502:LEU:HD11	2.33	0.44
1:A:632:ASP:CA	1:A:1033:MET:HE3	2.46	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
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:578:PHE:O	1:A:579:ARG:C	2.61	0.43
1:A:717:LEU:C	1:A:717:LEU:HD23	2.43	0.43
1:A:1029:ILE:C	1:A:1029:ILE:HD13	2.44	0.43
1:A:640:VAL:O	1:A:643:ILE:HG12	2.18	0.43
1:A:741:MET:C	1:A:743:GLN:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:SER:C	1:A:596:VAL:H	2.27	0.43
1:A:655:ASP:O	1:A:659:TYR:CD2	2.72	0.43
1:A:667:VAL:C	1:A:669:PHE:N	2.73	0.43
1:A:167:ASN:HD21	1:A:506:THR:H	1.66	0.43
1:A:677:LEU:O	1:A:678:ALA:C	2.61	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:907:LEU:HD22	1:A:994:VAL:HG21	2.00	0.42
1:A:919:GLU:O	1:A:921:PHE:N	2.51	0.42
1:A:393:VAL:HG23	1:A:393:VAL:O	2.20	0.42
1:A:499:ALA:C	1:A:501:LYS:N	2.76	0.42
1:A:701:SER:HB2	1:A:871:SER:HB3	2.02	0.42
1:A:905:GLU:H	1:A:905:GLU:HG3	1.68	0.42
1:A:655:ASP:O	1:A:659:TYR:HD2	2.02	0.42
1:A:785:VAL:O	1:A:786:PRO:C	2.62	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:1023:HIS:O	1:A:1024:THR:C	2.63	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:225:HIS:ND1	1:A:225:HIS:N	2.68	0.41
1:A:689:LYS:CE	1:A:728:MET:HG2	2.50	0.41
1:A:936:CYS:O	1:A:937:VAL:C	2.63	0.41
1:A:914:LYS:HA	1:A:914:LYS:HD3	1.78	0.41
1:A:682:LEU:HD21	1:A:720:TYR:HA	2.01	0.41
1:A:1043:THR:C	1:A:1045:LYS:N	2.78	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:N	1:A:838:LEU:HD22	2.35	0.41
1:A:944:ILE:O	1:A:947:ARG:HD3	2.21	0.41
1:A:1021:ARG:O	1:A:1023:HIS:N	2.53	0.41
1:A:863:CYS:O	1:A:864:LEU:C	2.64	0.41
1:A:192:ASP:OD1	1:A:192:ASP:C	2.63	0.41
1:A:623:ASP:OD1	1:A:623:ASP:C	2.64	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:630:LEU:HD23	1:A:630:LEU:HA	1.82	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

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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:568:THR:H	1:A:571:ASP:CG	2.29	0.41
1:A:874:ASP:CG	1:A:875:LYS:H	2.28	0.41
1:A:787:TYR:HA	1:A:870:ILE:HD11	2.02	0.40
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	2.03	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: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:1010:GLN:H	1:A:1010:GLN:HG3	1.75	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:652:GLU:O	1:A:653:ASP:C	2.64	0.40
1:A:780:PRO:O	1:A:781:GLU:C	2.65	0.40
1:A:861:ASP:C	1:A:862:LEU:HD22	2.47	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%)	1 11

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	PHE
1	A	579	ARG
1	A	615	GLU

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Mol	Chain	Res	Type
1	A	755	GLU
1	A	781	GLU
1	A	874	ASP
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%)	629 (85%)	113 (15%)	3 13

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	147	SER
1	A	158	ILE
1	A	163	THR
1	A	168	VAL
1	A	173	LEU
1	A	207	LEU
1	A	213	LYS
1	A	217	ASN
1	A	220	ILE
1	A	230	SER
1	A	235	VAL
1	A	252	MET
1	A	278	ASP
1	A	282	VAL
1	A	287	ILE
1	A	306	VAL
1	A	362	ARG
1	A	368	ILE
1	A	370	ILE
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	407	GLU
1	A	411	ASN
1	A	415	GLU

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Mol	Chain	Res	Type
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
1	A	477	ARG
1	A	486	GLN
1	A	503	THR
1	A	510	LYS
1	A	520	LEU
1	A	544	ARG
1	A	559	ILE
1	A	561	THR
1	A	568	THR
1	A	582	SER
1	A	583	LEU
1	A	587	LYS
1	A	595	SER
1	A	613	ARG
1	A	624	VAL
1	A	627	THR
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	739	ILE
1	A	745	VAL
1	A	747	LEU
1	A	748	ASP
1	A	749	ILE
1	A	750	LYS
1	A	759	VAL
1	A	767	LEU
1	A	796	LEU
1	A	799	GLU
1	A	803	VAL

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Mol	Chain	Res	Type
1	A	804	MET
1	A	827	THR
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	854	ILE
1	A	858	GLU
1	A	860	LEU
1	A	869	CYS
1	A	870	ILE
1	A	872	THR
1	A	876	ILE
1	A	878	MET
1	A	888	ILE
1	A	896	VAL
1	A	905	GLU
1	A	911	LEU
1	A	912	LYS
1	A	939	THR
1	A	949	ASN
1	A	952	ILE
1	A	960	LEU
1	A	963	ILE
1	A	967	HIS
1	A	1001	LYS
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	1051	ILE
1	A	1062	GLU
1	A	1076	ARG
1	A	1078	LYS
1	A	1082	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	153	GLN
1	A	169	HIS
1	A	217	ASN
1	A	268	GLN
1	A	295	HIS
1	A	304	HIS
1	A	391	GLN
1	A	432	GLN
1	A	498	ASN
1	A	550	GLN
1	A	577	HIS
1	A	634	ASN
1	A	710	GLN
1	A	735	GLN
1	A	743	GLN
1	A	762	GLN
1	A	769	GLN
1	A	776	ASN
1	A	846	GLN
1	A	893	GLN
1	A	948	HIS
1	A	949	ASN
1	A	1007	GLN
1	A	1010	GLN
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

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	-	25,25,25	2.84	5 (20%)	32,37,37	2.72	11 (34%)

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	-	-	4/14/14/14	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	7L0	NAD-NAM	-11.69	1.23	1.37
2	A	2095	7L0	CAA-CAB	-4.29	1.40	1.48
2	A	2095	7L0	CAC-NAD	3.05	1.41	1.36
2	A	2095	7L0	OAR-SAP	2.84	1.51	1.44
2	A	2095	7L0	OAS-SAP	2.69	1.50	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2095	7L0	CAN-NAM-NAD	7.86	109.13	100.67
2	A	2095	7L0	OAR-SAP-OAS	-6.42	107.11	117.99
2	A	2095	7L0	NAM-CAN-NAO	-4.90	110.14	116.67
2	A	2095	7L0	CAC-NAD-NAM	4.59	131.29	125.20
2	A	2095	7L0	CAQ-SAP-CAK	4.47	109.47	104.55
2	A	2095	7L0	CAL-CAK-SAP	3.74	122.02	119.02
2	A	2095	7L0	OAS-SAP-CAK	2.96	110.53	108.23
2	A	2095	7L0	CAJ-NAI-CAH	2.75	121.25	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	2095	7L0	OAR-SAP-CAK	2.49	110.16	108.23
2	A	2095	7L0	CAE-NAD-NAM	-2.43	108.10	111.33
2	A	2095	7L0	CAA-CAL-CAK	-2.02	118.18	119.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

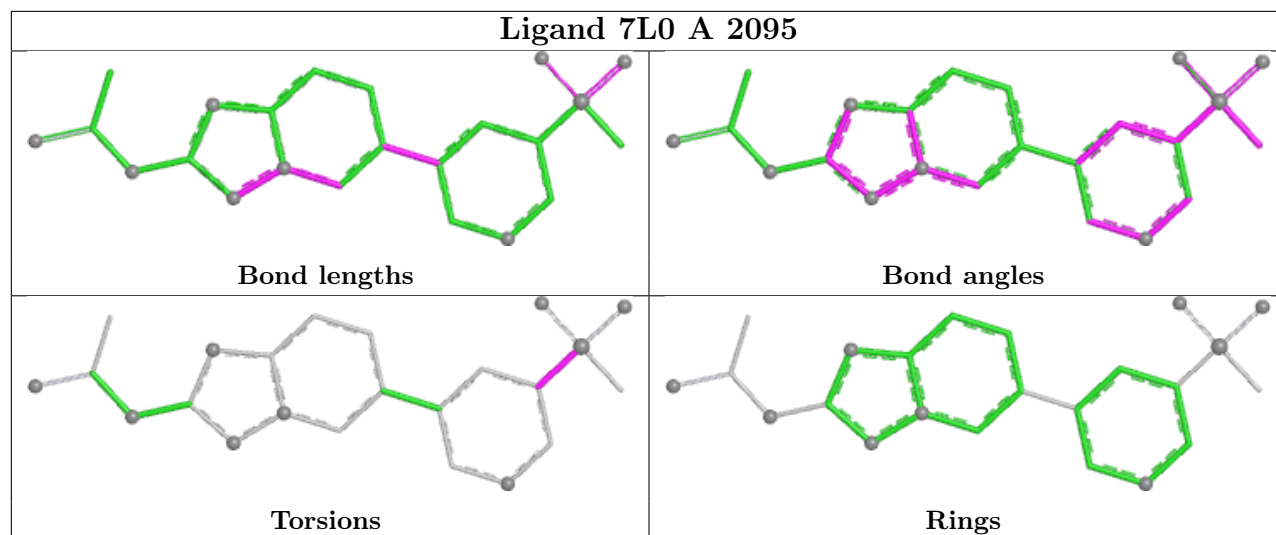
Mol	Chain	Res	Type	Atoms
2	A	2095	7L0	CAJ-CAK-SAP-OAR
2	A	2095	7L0	CAL-CAK-SAP-OAR
2	A	2095	7L0	CAL-CAK-SAP-CAQ
2	A	2095	7L0	CAJ-CAK-SAP-CAQ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2095	7L0	1	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 [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%)	0.15	5 (0%) 85 73	47, 66, 79, 90	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	895	THR	2.8
1	A	998	SER	2.6
1	A	1064	ALA	2.2
1	A	997	THR	2.2
1	A	860	LEU	2.1

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.

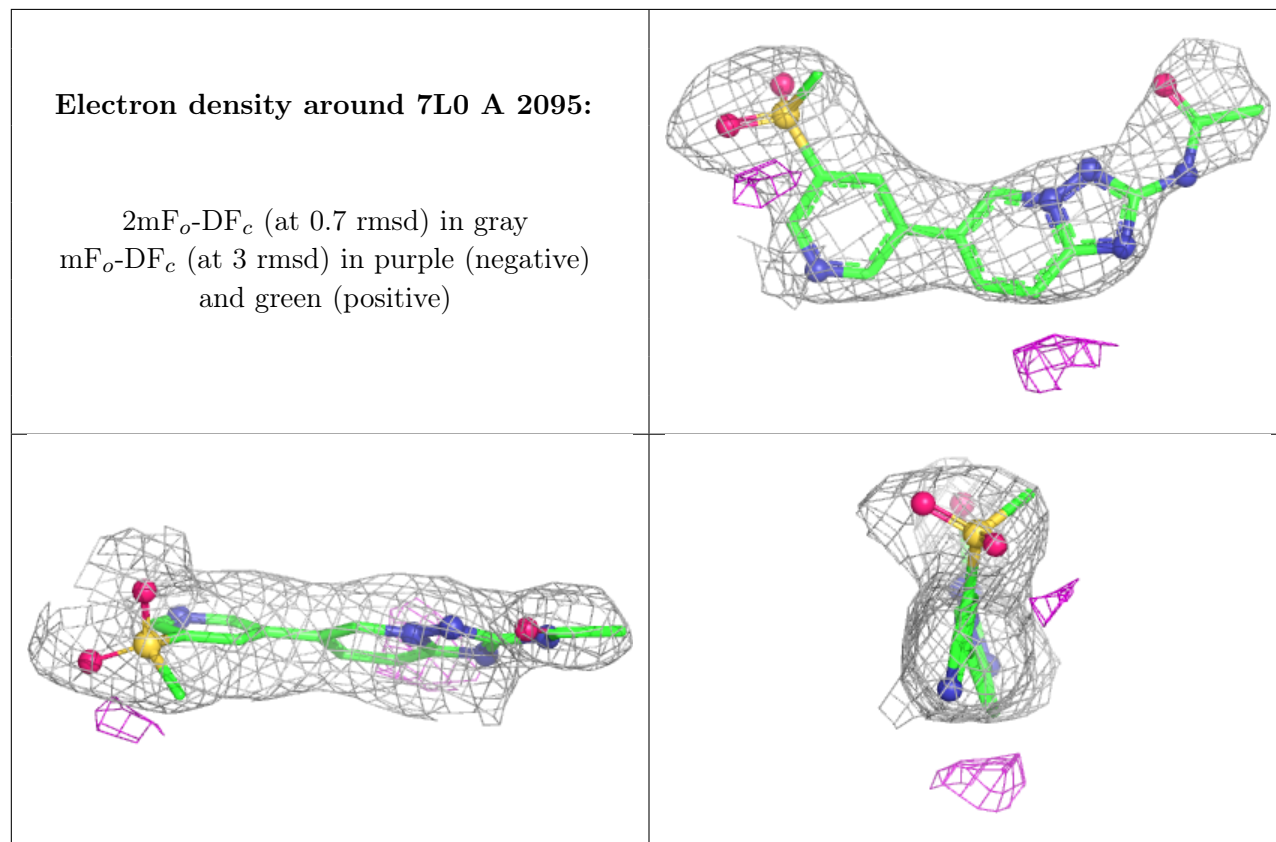
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	7L0	A	2095	23/23	0.89	0.11	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.