



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:14 AM UTC

PDB ID : 4ANW / pdb_00004anw
Title : Complexes of PI3Kgamma with isoform selective inhibitors.
Authors : Foster, P.G.; Lougheed, J.C.
Deposited on : 2012-03-22
Resolution : 2.31 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

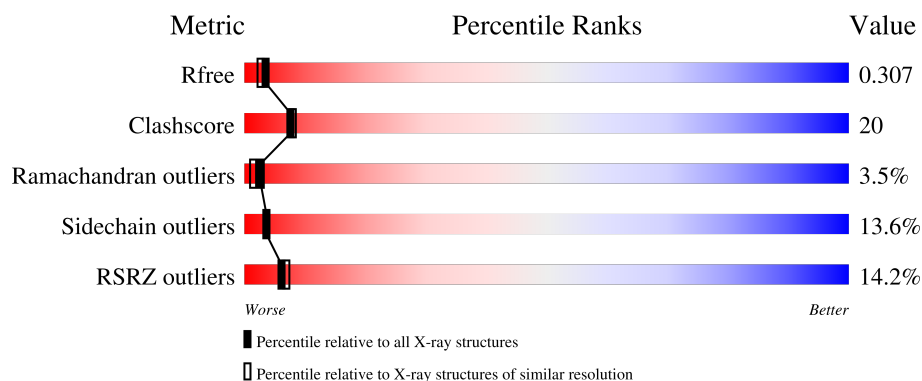
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	980	12% 47% 29% 8% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6888 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	833	Total	C	N	O	S	0	0	0
			6757	4334	1153	1235	35			

There are 21 discrepancies between the modelled and reference sequences:

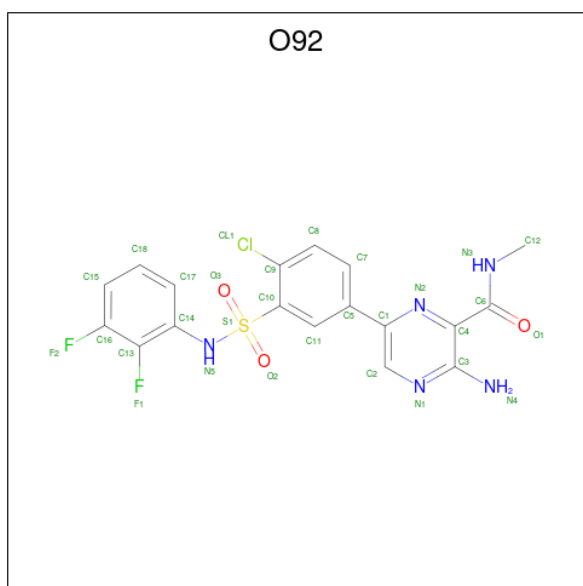
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	expression tag	UNP P48736
A	140	LEU	-	expression tag	UNP P48736
A	141	LEU	-	expression tag	UNP P48736
A	142	GLY	-	expression tag	UNP P48736
A	143	SER	-	expression tag	UNP P48736
A	1103	GLU	-	expression tag	UNP P48736
A	1104	PHE	-	expression tag	UNP P48736
A	1105	GLY	-	expression tag	UNP P48736
A	1106	LEU	-	expression tag	UNP P48736
A	1107	VAL	-	expression tag	UNP P48736
A	1108	PRO	-	expression tag	UNP P48736
A	1109	ARG	-	expression tag	UNP P48736
A	1110	GLY	-	expression tag	UNP P48736
A	1111	SER	-	expression tag	UNP P48736
A	1112	GLY	-	expression tag	UNP P48736
A	1113	HIS	-	expression tag	UNP P48736
A	1114	HIS	-	expression tag	UNP P48736
A	1115	HIS	-	expression tag	UNP P48736
A	1116	HIS	-	expression tag	UNP P48736
A	1117	HIS	-	expression tag	UNP P48736
A	1118	HIS	-	expression tag	UNP P48736

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 3-AMINO-6-{4-CHLORO-3-[(2,3-DIFLUOROPHENYL)SULFAMOYL]PHENYL}-N-METHYLPYRAZINE-2-CARBOXAMIDE (CCD ID: O92) (formula: C₁₈H₁₄ClF₂N₅O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	
			60	36	2	4	10	6	2	0
										1

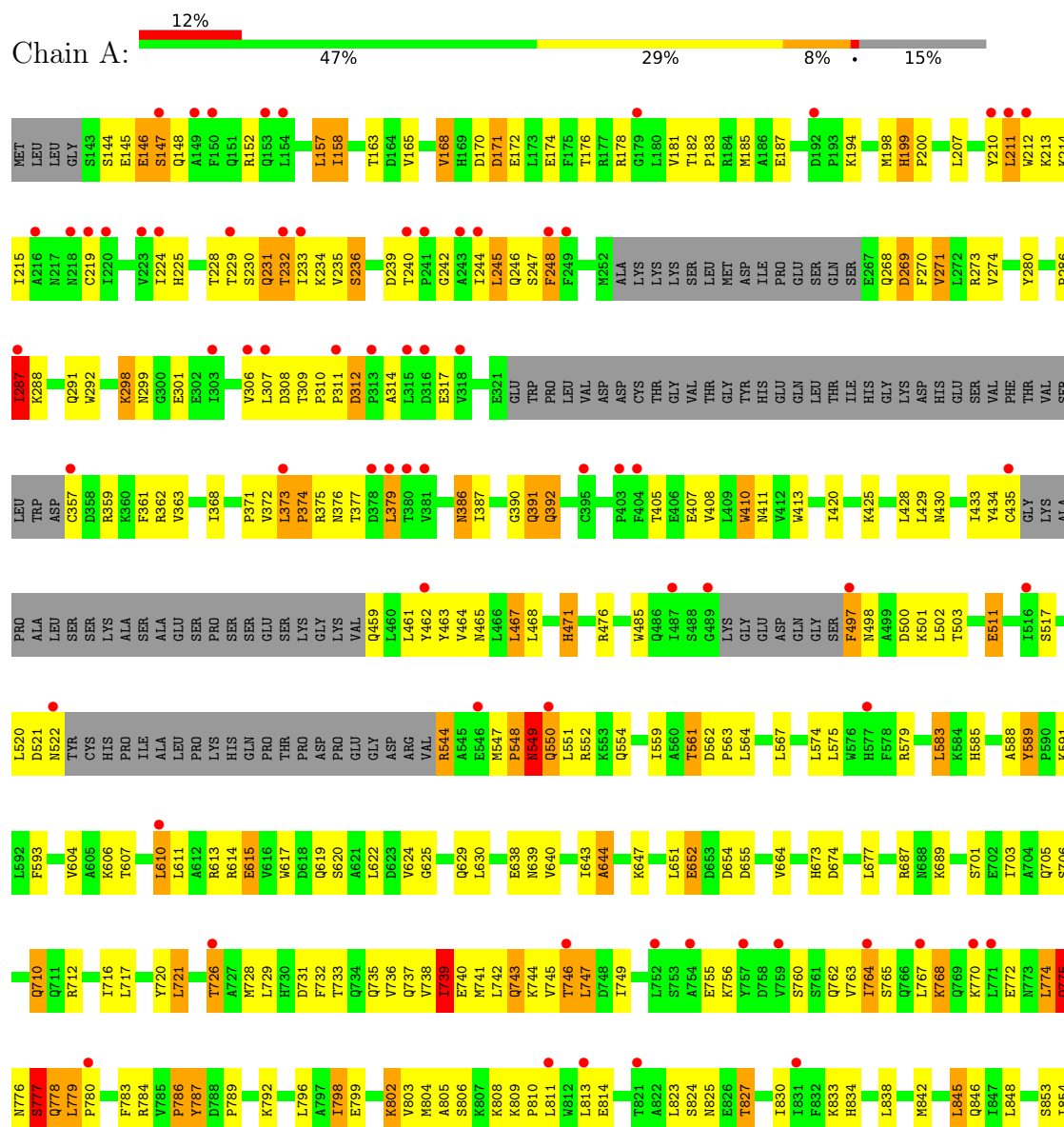
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total 66	O 66	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 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	143.42Å 68.53Å 106.26Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	71.43 – 2.31 71.43 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (71.43-2.31) 98.4 (71.43-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.296 0.246 , 0.307	Depositor DCC
R_{free} test set	2248 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.2	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	0.94	EDS
Total number of atoms	6888	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: O92, 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	1.15	12/6901 (0.2%)	1.22	33/9334 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	VAL	CA-CB	6.60	1.62	1.55
1	A	937	VAL	CA-CB	6.36	1.61	1.54
1	A	664	VAL	CA-CB	6.17	1.62	1.54
1	A	604	VAL	CA-CB	5.84	1.61	1.54
1	A	739	ILE	CA-CB	5.52	1.61	1.54
1	A	838	LEU	C-O	-5.42	1.16	1.24
1	A	716	ILE	CA-CB	5.29	1.61	1.54
1	A	881	ILE	CA-CB	5.29	1.59	1.53
1	A	846	GLN	CD-NE2	5.17	1.44	1.33
1	A	644	ALA	CA-CB	5.15	1.61	1.53
1	A	386	ASN	C-O	-5.12	1.17	1.24
1	A	845	LEU	CA-C	5.06	1.59	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	775	GLN	N-CA-C	9.47	121.54	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1039	MET	N-CA-C	7.51	118.77	110.13
1	A	967	HIS	CA-C-N	-7.19	108.76	121.70
1	A	967	HIS	C-N-CA	-7.19	108.76	121.70
1	A	915	SER	CA-C-N	6.81	127.37	119.47
1	A	915	SER	C-N-CA	6.81	127.37	119.47
1	A	777	SER	CA-C-N	6.80	133.93	121.70
1	A	777	SER	C-N-CA	6.80	133.93	121.70
1	A	677	LEU	N-CA-C	6.78	118.33	111.07
1	A	171	ASP	N-CA-C	6.73	121.33	113.18
1	A	786	PRO	N-CA-C	-6.60	101.54	111.57
1	A	585	HIS	CA-C-N	6.59	128.08	119.84
1	A	585	HIS	C-N-CA	6.59	128.08	119.84
1	A	710	GLN	N-CA-C	6.53	119.22	111.71
1	A	966	GLY	N-CA-C	6.27	128.04	113.18
1	A	1028	ILE	N-CA-C	6.07	116.84	110.72
1	A	1046	GLU	N-CA-C	6.06	117.97	111.36
1	A	308	ASP	N-CA-C	5.88	116.00	108.24
1	A	964	ASP	N-CA-C	5.72	118.17	111.02
1	A	967	HIS	O-C-N	-5.60	114.04	123.00
1	A	802	LYS	N-CA-C	5.59	116.76	108.60
1	A	624	VAL	N-CA-C	5.55	116.18	110.36
1	A	949	ASN	N-CA-C	5.39	119.61	113.19
1	A	312	ASP	CA-C-N	5.19	124.91	119.82
1	A	312	ASP	C-N-CA	5.19	124.91	119.82
1	A	199	HIS	CA-C-N	-5.11	114.67	119.89
1	A	199	HIS	C-N-CA	-5.11	114.67	119.89
1	A	589	TYR	CA-C-N	5.08	124.52	119.24
1	A	589	TYR	C-N-CA	5.08	124.52	119.24
1	A	848	LEU	N-CA-C	5.07	116.88	111.36
1	A	966	GLY	CA-C-N	5.03	130.75	121.70
1	A	966	GLY	C-N-CA	5.03	130.75	121.70
1	A	158	ILE	N-CA-C	5.01	115.24	110.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1039	MET	Peptide
1	A	410	TRP	Peptide
1	A	965	PHE	Peptide

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	6757	0	6789	275	0
2	A	5	0	0	0	0
3	A	60	0	28	8	0
4	A	66	0	0	2	0
All	All	6888	0	6817	275	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 20.

All (275) 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:777:SER:CB	1:A:778:GLN:HB2	1.59	1.31
1:A:967:HIS:H	1:A:968:ILE:HA	0.99	1.15
1:A:777:SER:HB3	1:A:778:GLN:CB	1.76	1.14
1:A:966:GLY:HA3	1:A:967:HIS:HB2	1.31	1.08
1:A:967:HIS:N	1:A:968:ILE:HA	1.61	1.02
1:A:210:TYR:O	1:A:211:LEU:HB2	1.62	0.97
1:A:947:ARG:NH2	1:A:963:ILE:O	1.98	0.95
1:A:775:GLN:HB3	1:A:776:ASN:HB2	1.47	0.95
1:A:428:LEU:HD23	1:A:467:LEU:HD12	1.47	0.95
1:A:673:HIS:HD2	1:A:712:ARG:HE	1.12	0.93
1:A:777:SER:HB3	1:A:778:GLN:HB2	0.90	0.89
1:A:430:ASN:HD22	1:A:465:ASN:ND2	1.72	0.86
1:A:652:GLU:OE2	1:A:654:ASP:HB3	1.76	0.86
1:A:298:LYS:NZ	1:A:299:ASN:HD21	1.77	0.82
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.64	0.80
1:A:145:GLU:HA	1:A:146:GLU:O	1.82	0.79
1:A:219:CYS:SG	1:A:234:LYS:HG3	2.23	0.79
1:A:966:GLY:CA	1:A:967:HIS:HB2	2.12	0.78
1:A:298:LYS:HZ1	1:A:299:ASN:HD21	1.31	0.77
1:A:551:LEU:O	1:A:554:GLN:HB2	1.85	0.77
1:A:804:MET:HE2	3:A:1189[A]:O92:C17	2.15	0.77
1:A:428:LEU:CD2	1:A:467:LEU:HD12	2.15	0.76
1:A:772:GLU:O	1:A:776:ASN:HB3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:O	1:A:1042:LEU:CD1	2.34	0.76
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.27	0.74
1:A:207:LEU:HD21	1:A:211:LEU:HB3	1.69	0.74
1:A:967:HIS:H	1:A:968:ILE:CA	1.92	0.73
1:A:928:PHE:O	1:A:932:CYS:HB2	1.88	0.73
1:A:219:CYS:SG	1:A:234:LYS:CG	2.77	0.73
1:A:405:THR:HG23	1:A:407:GLU:O	1.88	0.73
1:A:814:GLU:OE1	1:A:827:THR:HG21	1.89	0.73
1:A:430:ASN:HD22	1:A:465:ASN:HD21	1.32	0.72
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.37	0.72
1:A:212:TRP:HA	1:A:215:ILE:HD12	1.72	0.71
1:A:172:GLU:HG3	1:A:471:HIS:CD2	2.25	0.70
1:A:271:VAL:HG13	1:A:310:PRO:HG3	1.74	0.70
1:A:497:PHE:O	1:A:1042:LEU:HD13	1.91	0.69
1:A:146:GLU:O	1:A:148:GLN:N	2.25	0.69
1:A:689:LYS:HG2	1:A:728:MET:SD	2.32	0.69
1:A:476:ARG:O	1:A:520:LEU:HD23	1.93	0.69
1:A:774:LEU:O	1:A:778:GLN:HB3	1.93	0.68
1:A:997:THR:OG1	1:A:1003:SER:HB2	1.92	0.68
1:A:615:GLU:O	1:A:619:GLN:HG3	1.94	0.67
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.74	0.67
1:A:701:SER:O	1:A:705:GLN:HG2	1.95	0.67
1:A:168:VAL:CG1	1:A:170:ASP:O	2.43	0.67
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.77	0.67
1:A:743:GLN:O	1:A:747:LEU:HD22	1.94	0.67
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.77	0.66
1:A:673:HIS:CD2	1:A:712:ARG:HE	2.04	0.66
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.76	0.66
1:A:244:ILE:HD11	1:A:287:ILE:HG12	1.78	0.65
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.77	0.65
1:A:762:GLN:HA	1:A:765:SER:HB3	1.79	0.65
1:A:770:LYS:O	1:A:774:LEU:HB2	1.96	0.65
1:A:833:LYS:NZ	3:A:1189[B]:O92:O3	2.23	0.64
1:A:579:ARG:HD2	1:A:610:LEU:HD22	1.79	0.64
1:A:887:THR:HG22	1:A:890:LYS:H	1.63	0.64
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.79	0.64
1:A:617:TRP:O	1:A:620:SER:OG	2.15	0.62
1:A:968:ILE:HG12	1:A:968:ILE:O	1.98	0.62
1:A:224:ILE:HG22	1:A:225:HIS:N	2.15	0.62
1:A:240:THR:HG22	1:A:242:GLY:H	1.64	0.62
1:A:548:PRO:O	1:A:549:ASN:C	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:HIS:HB2	1:A:876:ILE:CD1	2.30	0.61
1:A:933:ALA:O	1:A:937:VAL:HG23	2.00	0.61
1:A:174:GLU:O	1:A:178:ARG:HG3	1.99	0.61
1:A:361:PHE:HA	1:A:420:ILE:CD1	2.30	0.61
1:A:561:THR:CG2	1:A:591:LYS:HE2	2.31	0.61
1:A:804:MET:HB2	1:A:810:PRO:HD2	1.82	0.61
1:A:993:PHE:O	1:A:994:VAL:HG23	2.01	0.61
1:A:471:HIS:CD2	1:A:471:HIS:H	2.17	0.60
1:A:497:PHE:O	1:A:1042:LEU:HD11	2.01	0.60
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.31	0.60
1:A:777:SER:CB	1:A:778:GLN:CB	2.55	0.60
1:A:357:CYS:SG	1:A:359:ARG:HG2	2.42	0.60
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.84	0.59
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.36	0.59
1:A:1003:SER:O	1:A:1007:GLN:HB2	2.00	0.59
1:A:547:MET:O	1:A:548:PRO:C	2.42	0.59
1:A:887:THR:HG23	1:A:889:ALA:H	1.66	0.59
1:A:181:VAL:HG13	1:A:185:MET:HE3	1.85	0.59
1:A:210:TYR:O	1:A:211:LEU:CB	2.43	0.59
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.01	0.59
1:A:706:SER:O	1:A:710:GLN:HB3	2.02	0.59
1:A:967:HIS:N	1:A:968:ILE:CA	2.53	0.59
1:A:1060:ASN:OD1	1:A:1062:GLU:HB2	2.02	0.58
1:A:434:TYR:HA	1:A:459:GLN:O	2.04	0.58
1:A:246:GLN:C	1:A:248:PHE:H	2.12	0.58
1:A:741:MET:HE1	1:A:778:GLN:O	2.03	0.58
1:A:165:VAL:HG12	1:A:165:VAL:O	2.04	0.57
1:A:298:LYS:NZ	1:A:299:ASN:ND2	2.51	0.57
1:A:804:MET:HE2	3:A:1189[B]:O92:C13	2.34	0.57
1:A:911:LEU:O	1:A:915:SER:OG	2.22	0.57
1:A:232:THR:CG2	1:A:233:ILE:N	2.67	0.57
1:A:230:SER:O	1:A:231:GLN:HB2	2.05	0.57
1:A:742:LEU:HD22	1:A:813:LEU:HD11	1.87	0.56
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.39	0.56
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.05	0.56
1:A:168:VAL:HG13	1:A:170:ASP:H	1.70	0.56
1:A:182:THR:HB	1:A:183:PRO:CD	2.36	0.56
1:A:373:LEU:O	1:A:374:PRO:C	2.49	0.56
1:A:371:PRO:HG2	1:A:511:GLU:O	2.06	0.55
1:A:842:MET:HE3	1:A:870:ILE:HA	1.87	0.55
1:A:1002:THR:HG22	1:A:1003:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.89	0.55
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.88	0.55
1:A:498:ASN:HD22	1:A:1041:GLN:HE22	1.54	0.55
1:A:775:GLN:NE2	1:A:798:ILE:HD11	2.21	0.55
1:A:236:SER:O	1:A:287:ILE:HD11	2.07	0.54
1:A:273:ARG:HG3	1:A:280:TYR:CE2	2.43	0.54
1:A:742:LEU:O	1:A:746:THR:HG22	2.06	0.54
1:A:1032:SER:O	1:A:1036:MET:HG3	2.08	0.54
1:A:428:LEU:CD2	1:A:467:LEU:CD1	2.86	0.54
1:A:804:MET:HE2	3:A:1189[A]:O92:C18	2.38	0.54
1:A:583:LEU:HD12	1:A:613:ARG:HD3	1.88	0.54
1:A:738:VAL:CG1	1:A:742:LEU:HD12	2.38	0.54
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.43	0.53
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.09	0.53
1:A:425:LYS:NZ	4:A:2022:HOH:O	2.28	0.53
1:A:625:GLY:O	1:A:629:GLN:HG3	2.08	0.53
1:A:798:ILE:HD12	1:A:798:ILE:H	1.73	0.53
1:A:362:ARG:H	1:A:522:ASN:HD21	1.57	0.53
1:A:1041:GLN:HA	1:A:1041:GLN:NE2	2.23	0.53
1:A:145:GLU:CA	1:A:146:GLU:O	2.56	0.52
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.91	0.52
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.44	0.52
1:A:561:THR:HG22	1:A:591:LYS:HE2	1.90	0.52
1:A:735:GLN:O	1:A:739:ILE:CD1	2.58	0.52
1:A:804:MET:HE2	3:A:1189[B]:O92:F1	1.97	0.52
1:A:198:MET:O	1:A:199:HIS:C	2.53	0.52
1:A:547:MET:HE2	1:A:552:ARG:N	2.25	0.52
1:A:291:GLN:NE2	1:A:654:ASP:OD1	2.41	0.52
1:A:168:VAL:CG1	1:A:170:ASP:H	2.23	0.52
1:A:212:TRP:C	1:A:214:LYS:H	2.17	0.51
1:A:224:ILE:HG22	1:A:225:HIS:H	1.75	0.51
1:A:317:GLU:O	1:A:726:THR:HG23	2.10	0.51
1:A:786:PRO:O	1:A:787:TYR:CG	2.64	0.51
1:A:853:SER:O	1:A:857:THR:HG23	2.10	0.51
1:A:992:LEU:O	1:A:995:MET:HB2	2.11	0.51
1:A:833:LYS:NZ	3:A:1189[A]:O92:O3	2.28	0.51
1:A:207:LEU:C	1:A:207:LEU:HD23	2.35	0.51
1:A:168:VAL:HG11	1:A:170:ASP:O	2.10	0.51
1:A:834:HIS:CA	1:A:876:ILE:HD12	2.40	0.51
1:A:246:GLN:C	1:A:248:PHE:N	2.69	0.50
1:A:1049:GLU:HG3	1:A:1049:GLU:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:GLU:O	1:A:744:LYS:HG3	2.11	0.50
1:A:163:THR:O	1:A:165:VAL:HG23	2.11	0.50
1:A:639:ASN:O	1:A:643:ILE:HG23	2.12	0.50
1:A:834:HIS:CB	1:A:876:ILE:HD12	2.41	0.50
1:A:775:GLN:HE22	1:A:798:ILE:HD11	1.76	0.49
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.94	0.49
1:A:559:ILE:O	1:A:559:ILE:CG2	2.60	0.49
1:A:760:SER:OG	1:A:763:VAL:HG23	2.12	0.49
1:A:181:VAL:O	1:A:185:MET:HG3	2.13	0.49
1:A:772:GLU:C	1:A:774:LEU:H	2.20	0.49
1:A:1073:GLU:HA	1:A:1073:GLU:OE1	2.12	0.48
1:A:187:GLU:OE2	1:A:687:ARG:HB2	2.13	0.48
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.96	0.48
1:A:567:LEU:HD21	1:A:591:LYS:HD3	1.95	0.48
1:A:224:ILE:CG2	1:A:225:HIS:N	2.77	0.48
1:A:739:ILE:O	1:A:743:GLN:HB2	2.13	0.48
1:A:824:SER:OG	1:A:825:ASN:N	2.46	0.48
1:A:219:CYS:SG	1:A:234:LYS:HG2	2.51	0.48
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.12	0.48
1:A:269:ASP:OD1	1:A:269:ASP:N	2.47	0.48
1:A:583:LEU:HD22	1:A:589:TYR:CZ	2.48	0.48
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.14	0.48
1:A:298:LYS:HZ1	1:A:299:ASN:ND2	2.06	0.48
1:A:904:ASP:N	1:A:904:ASP:OD1	2.46	0.47
1:A:1002:THR:CG2	1:A:1003:SER:N	2.77	0.47
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.79	0.47
1:A:717:LEU:HG	1:A:721:LEU:HD22	1.96	0.47
1:A:746:THR:HB	1:A:811:LEU:HG	1.96	0.47
1:A:270:PHE:HB3	1:A:307:LEU:HD11	1.96	0.47
1:A:548:PRO:O	1:A:550:GLN:N	2.47	0.47
1:A:224:ILE:CG2	1:A:225:HIS:H	2.28	0.47
1:A:411:ASN:CG	1:A:411:ASN:O	2.58	0.47
1:A:391:GLN:HE21	1:A:391:GLN:HB3	1.57	0.47
1:A:775:GLN:CB	1:A:776:ASN:HB2	2.31	0.47
1:A:606:LYS:O	1:A:610:LEU:HD23	2.14	0.47
1:A:273:ARG:HB3	1:A:306:VAL:HG12	1.98	0.46
1:A:207:LEU:HD12	1:A:288:LYS:HB2	1.97	0.46
1:A:246:GLN:O	1:A:248:PHE:N	2.40	0.46
1:A:430:ASN:ND2	1:A:465:ASN:HD21	2.06	0.46
1:A:784:ARG:HD3	1:A:789:PRO:O	2.16	0.46
1:A:1009:PHE:CE1	1:A:1072:ILE:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:CD1	1:A:387:ILE:HD11	2.51	0.46
1:A:865:LEU:HD12	1:A:961:PHE:CD1	2.51	0.46
1:A:999:GLY:O	1:A:1000:LYS:HB2	2.16	0.46
1:A:375:ARG:HG3	1:A:376:ASN:H	1.80	0.46
1:A:742:LEU:HD22	1:A:813:LEU:CD1	2.45	0.45
1:A:232:THR:HG22	1:A:233:ILE:N	2.31	0.45
1:A:298:LYS:HZ3	1:A:299:ASN:HD21	1.59	0.45
1:A:640:VAL:O	1:A:643:ILE:HG12	2.17	0.45
1:A:735:GLN:O	1:A:739:ILE:HD13	2.16	0.45
1:A:171:ASP:HB3	1:A:471:HIS:HE1	1.82	0.45
1:A:286:PRO:O	1:A:287:ILE:C	2.58	0.45
1:A:182:THR:HB	1:A:183:PRO:HD3	1.98	0.45
1:A:629:GLN:HG2	1:A:1029:ILE:HG12	1.99	0.45
1:A:157:LEU:HD11	1:A:733:THR:HA	1.99	0.45
1:A:413:TRP:HH2	1:A:521:ASP:HB2	1.82	0.45
1:A:559:ILE:O	1:A:559:ILE:HG22	2.17	0.45
1:A:862:LEU:HD21	1:A:1016:ALA:HB2	1.99	0.45
1:A:562:ASP:HB2	1:A:563:PRO:HD2	1.99	0.44
1:A:741:MET:O	1:A:745:VAL:HG23	2.18	0.44
1:A:799:GLU:CD	1:A:799:GLU:H	2.24	0.44
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.98	0.44
1:A:500:ASP:O	1:A:503:THR:HG22	2.16	0.44
1:A:551:LEU:HD22	1:A:574:LEU:HD11	1.98	0.44
1:A:245:LEU:O	1:A:248:PHE:HB3	2.17	0.44
1:A:775:GLN:NE2	1:A:796:LEU:HB2	2.33	0.44
1:A:873:GLY:C	1:A:876:ILE:HG22	2.42	0.44
1:A:1036:MET:HG2	1:A:1042:LEU:HD21	2.00	0.44
1:A:777:SER:OG	1:A:778:GLN:HB2	2.12	0.44
1:A:198:MET:SD	1:A:271:VAL:HG11	2.58	0.44
1:A:777:SER:CA	1:A:778:GLN:HB2	2.39	0.44
1:A:732:PHE:O	1:A:736:VAL:HG23	2.16	0.44
1:A:199:HIS:O	1:A:200:PRO:C	2.59	0.43
1:A:497:PHE:CD1	1:A:497:PHE:N	2.85	0.43
1:A:548:PRO:CG	1:A:551:LEU:HD12	2.42	0.43
1:A:550:GLN:HE21	1:A:550:GLN:HB3	1.68	0.43
1:A:239:ASP:O	1:A:287:ILE:HG13	2.18	0.43
1:A:735:GLN:O	1:A:739:ILE:HD12	2.18	0.43
1:A:548:PRO:O	1:A:551:LEU:N	2.51	0.43
1:A:559:ILE:HG12	1:A:588:ALA:HB2	2.00	0.43
1:A:809:LYS:N	1:A:810:PRO:HD3	2.34	0.43
1:A:993:PHE:O	1:A:994:VAL:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASN:HB2	1:A:430:ASN:HB3	1.99	0.43
1:A:804:MET:O	1:A:806:SER:N	2.50	0.43
1:A:720:TYR:OH	4:A:2007:HOH:O	2.20	0.43
1:A:1082:VAL:HA	1:A:1085:ASN:HB2	2.00	0.43
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.19	0.43
1:A:935:TYR:O	1:A:939:THR:HG23	2.19	0.42
1:A:158:ILE:HG23	1:A:703:ILE:HD13	2.01	0.42
1:A:547:MET:O	1:A:549:ASN:N	2.52	0.42
1:A:1043:THR:HB	1:A:1047:ASP:H	1.84	0.42
1:A:361:PHE:CA	1:A:420:ILE:CD1	2.97	0.42
1:A:738:VAL:HG21	1:A:783:PHE:CD1	2.54	0.42
1:A:1009:PHE:HE1	1:A:1072:ILE:HD13	1.85	0.42
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.55	0.42
1:A:630:LEU:HB2	1:A:644:ALA:HB2	2.02	0.42
1:A:390:GLY:C	1:A:392:GLN:H	2.28	0.41
1:A:775:GLN:H	1:A:776:ASN:HB3	1.84	0.41
1:A:804:MET:HB3	3:A:1189[A]:O92:H18	2.01	0.41
1:A:210:TYR:CD2	1:A:211:LEU:HD13	2.55	0.41
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	2.01	0.41
1:A:467:LEU:HB2	1:A:476:ARG:HH21	1.85	0.41
1:A:768:LYS:HG2	1:A:798:ILE:CG2	2.51	0.41
1:A:562:ASP:OD2	1:A:1052:ARG:HD2	2.21	0.41
1:A:144:SER:OG	1:A:146:GLU:HB3	2.20	0.41
1:A:270:PHE:HB3	1:A:307:LEU:CD1	2.51	0.41
1:A:310:PRO:HA	1:A:311:PRO:HD2	1.93	0.41
1:A:779:LEU:HD13	1:A:780:PRO:HD2	2.02	0.41
1:A:911:LEU:HD12	1:A:911:LEU:HA	2.00	0.41
1:A:1073:GLU:O	1:A:1074:VAL:C	2.63	0.41
1:A:361:PHE:CA	1:A:420:ILE:HD12	2.51	0.41
1:A:607:THR:HA	1:A:610:LEU:CD2	2.51	0.41
1:A:953:MET:HE1	3:A:1189[B]:O92:C6	2.51	0.41
1:A:1003:SER:HB3	1:A:1006:PHE:H	1.85	0.41
1:A:1008:LYS:O	1:A:1011:ASP:HB3	2.20	0.41
1:A:544:ARG:CZ	1:A:544:ARG:HA	2.51	0.41
1:A:995:MET:O	1:A:1005:HIS:HB2	2.21	0.41
1:A:731:ASP:O	1:A:735:GLN:HG3	2.21	0.40
1:A:1043:THR:HG22	1:A:1045:LYS:H	1.87	0.40
1:A:1059:LYS:HD3	1:A:1059:LYS:HA	1.77	0.40
1:A:317:GLU:O	1:A:726:THR:CG2	2.69	0.40
1:A:233:ILE:CD1	1:A:248:PHE:HB2	2.51	0.40
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:THR:HG22	1:A:883:LYS:NZ	2.35	0.40
1:A:176:THR:HG23	1:A:674:ASP:HB2	2.02	0.40
1:A:359:ARG:HG3	1:A:420:ILE:HD13	2.02	0.40
1:A:462:TYR:HA	1:A:485:TRP:O	2.22	0.40
1:A:764:ILE:H	1:A:764:ILE:HG13	1.67	0.40
1:A:775:GLN:HB3	1:A:776:ASN:CB	2.33	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	819/980 (84%)	720 (88%)	70 (8%)	29 (4%)	3 1

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	147	SER
1	A	211	LEU
1	A	374	PRO
1	A	778	GLN
1	A	805	ALA
1	A	967	HIS
1	A	994	VAL
1	A	1000	LYS
1	A	1040	PRO
1	A	213	LYS
1	A	247	SER
1	A	777	SER
1	A	798	ILE
1	A	896	VAL

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Mol	Chain	Res	Type
1	A	901	ALA
1	A	966	GLY
1	A	1079	GLY
1	A	231	GLN
1	A	287	ILE
1	A	898	ASN
1	A	1085	ASN
1	A	248	PHE
1	A	549	ASN
1	A	905	GLU
1	A	1001	LYS
1	A	379	LEU
1	A	895	THR
1	A	548	PRO

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	749/874 (86%)	647 (86%)	102 (14%)	3 3

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	152	ARG
1	A	157	LEU
1	A	168	VAL
1	A	194	LYS
1	A	228	THR
1	A	229	THR
1	A	232	THR
1	A	235	VAL
1	A	236	SER
1	A	245	LEU
1	A	268	GLN

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Mol	Chain	Res	Type
1	A	269	ASP
1	A	271	VAL
1	A	287	ILE
1	A	298	LYS
1	A	301	GLU
1	A	309	THR
1	A	372	VAL
1	A	373	LEU
1	A	377	THR
1	A	379	LEU
1	A	391	GLN
1	A	392	GLN
1	A	408	VAL
1	A	410	TRP
1	A	467	LEU
1	A	471	HIS
1	A	497	PHE
1	A	502	LEU
1	A	511	GLU
1	A	517	SER
1	A	544	ARG
1	A	549	ASN
1	A	550	GLN
1	A	561	THR
1	A	575	LEU
1	A	583	LEU
1	A	610	LEU
1	A	614	ARG
1	A	615	GLU
1	A	638	GLU
1	A	652	GLU
1	A	721	LEU
1	A	726	THR
1	A	729	LEU
1	A	737	GLN
1	A	739	ILE
1	A	743	GLN
1	A	746	THR
1	A	747	LEU
1	A	749	ILE
1	A	755	GLU
1	A	756	LYS

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Mol	Chain	Res	Type
1	A	764	ILE
1	A	768	LYS
1	A	774	LEU
1	A	775	GLN
1	A	779	LEU
1	A	787	TYR
1	A	792	LYS
1	A	802	LYS
1	A	808	LYS
1	A	823	LEU
1	A	827	THR
1	A	830	ILE
1	A	845	LEU
1	A	876	ILE
1	A	886	THR
1	A	887	THR
1	A	890	LYS
1	A	894	SER
1	A	895	THR
1	A	899	THR
1	A	904	ASP
1	A	905	GLU
1	A	908	ASN
1	A	911	LEU
1	A	912	LYS
1	A	915	SER
1	A	919	GLU
1	A	949	ASN
1	A	959	ASN
1	A	967	HIS
1	A	1000	LYS
1	A	1007	GLN
1	A	1024	THR
1	A	1029	ILE
1	A	1039	MET
1	A	1041	GLN
1	A	1042	LEU
1	A	1043	THR
1	A	1045	LYS
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG

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Mol	Chain	Res	Type
1	A	1059	LYS
1	A	1065	LYS
1	A	1066	LYS
1	A	1072	ILE
1	A	1078	LYS
1	A	1087	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	268	GLN
1	A	295	HIS
1	A	299	ASN
1	A	376	ASN
1	A	386	ASN
1	A	388	GLN
1	A	389	HIS
1	A	391	GLN
1	A	465	ASN
1	A	471	HIS
1	A	522	ASN
1	A	549	ASN
1	A	550	GLN
1	A	554	GLN
1	A	565	ASN
1	A	629	GLN
1	A	646	GLN
1	A	662	GLN
1	A	673	HIS
1	A	705	GLN
1	A	775	GLN
1	A	778	GLN
1	A	893	GLN
1	A	908	ASN
1	A	949	ASN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN
1	A	1085	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	O92	A	1189[A]	-	32,32,32	2.54	8 (25%)	45,47,47	2.18	9 (20%)
3	O92	A	1189[B]	-	32,32,32	2.48	7 (21%)	45,47,47	2.12	9 (20%)
2	SO4	A	1188	-	4,4,4	0.43	0	6,6,6	0.76	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
3	O92	A	1189[A]	-	-	7/21/21/21	0/3/3/3
3	O92	A	1189[B]	-	-	2/21/21/21	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1189[B]	O92	O2-S1	7.86	1.52	1.43
3	A	1189[A]	O92	O2-S1	7.48	1.52	1.43
3	A	1189[A]	O92	C5-C1	-5.62	1.40	1.49
3	A	1189[B]	O92	C5-C1	-5.49	1.40	1.49
3	A	1189[B]	O92	O3-S1	5.21	1.49	1.43
3	A	1189[B]	O92	C10-S1	5.19	1.84	1.77
3	A	1189[A]	O92	O3-S1	5.02	1.49	1.43
3	A	1189[A]	O92	C18-C17	4.81	1.47	1.38
3	A	1189[A]	O92	C14-N5	-4.78	1.35	1.42
3	A	1189[A]	O92	C10-S1	4.41	1.83	1.77
3	A	1189[B]	O92	C14-N5	-4.40	1.35	1.42
3	A	1189[A]	O92	C4-C6	3.04	1.55	1.50
3	A	1189[B]	O92	C4-C6	2.68	1.54	1.50
3	A	1189[A]	O92	C17-C14	2.31	1.43	1.39
3	A	1189[B]	O92	C6-N3	2.02	1.36	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1189[B]	O92	O3-S1-O2	-10.56	106.70	119.52
3	A	1189[A]	O92	O3-S1-O2	-9.25	108.29	119.52
3	A	1189[A]	O92	C13-C14-N5	5.88	127.54	120.73
3	A	1189[A]	O92	C15-C18-C17	-3.27	116.03	120.24
3	A	1189[B]	O92	O3-S1-N5	2.89	113.79	106.74
3	A	1189[A]	O92	F1-C13-C14	2.64	122.48	118.28
3	A	1189[B]	O92	O3-S1-C10	2.62	112.00	107.68
3	A	1189[A]	O92	C2-N1-C3	2.53	121.08	118.64
3	A	1189[A]	O92	C17-C14-N5	-2.52	116.05	120.92
3	A	1189[B]	O92	C13-C14-N5	-2.45	117.89	120.73
3	A	1189[B]	O92	C2-N1-C3	2.37	120.94	118.64
3	A	1189[B]	O92	C4-C3-N4	-2.28	120.29	122.90
3	A	1189[A]	O92	O1-C6-N3	2.24	125.98	122.67
3	A	1189[A]	O92	C18-C17-C14	2.22	123.20	118.69
3	A	1189[A]	O92	C4-C3-N4	-2.09	120.51	122.90
3	A	1189[B]	O92	C10-S1-N5	-2.07	104.86	107.30
3	A	1189[B]	O92	C18-C17-C14	2.07	122.89	118.69
3	A	1189[B]	O92	O2-S1-C10	2.02	111.03	107.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1189[A]	O92	C9-C10-S1-N5

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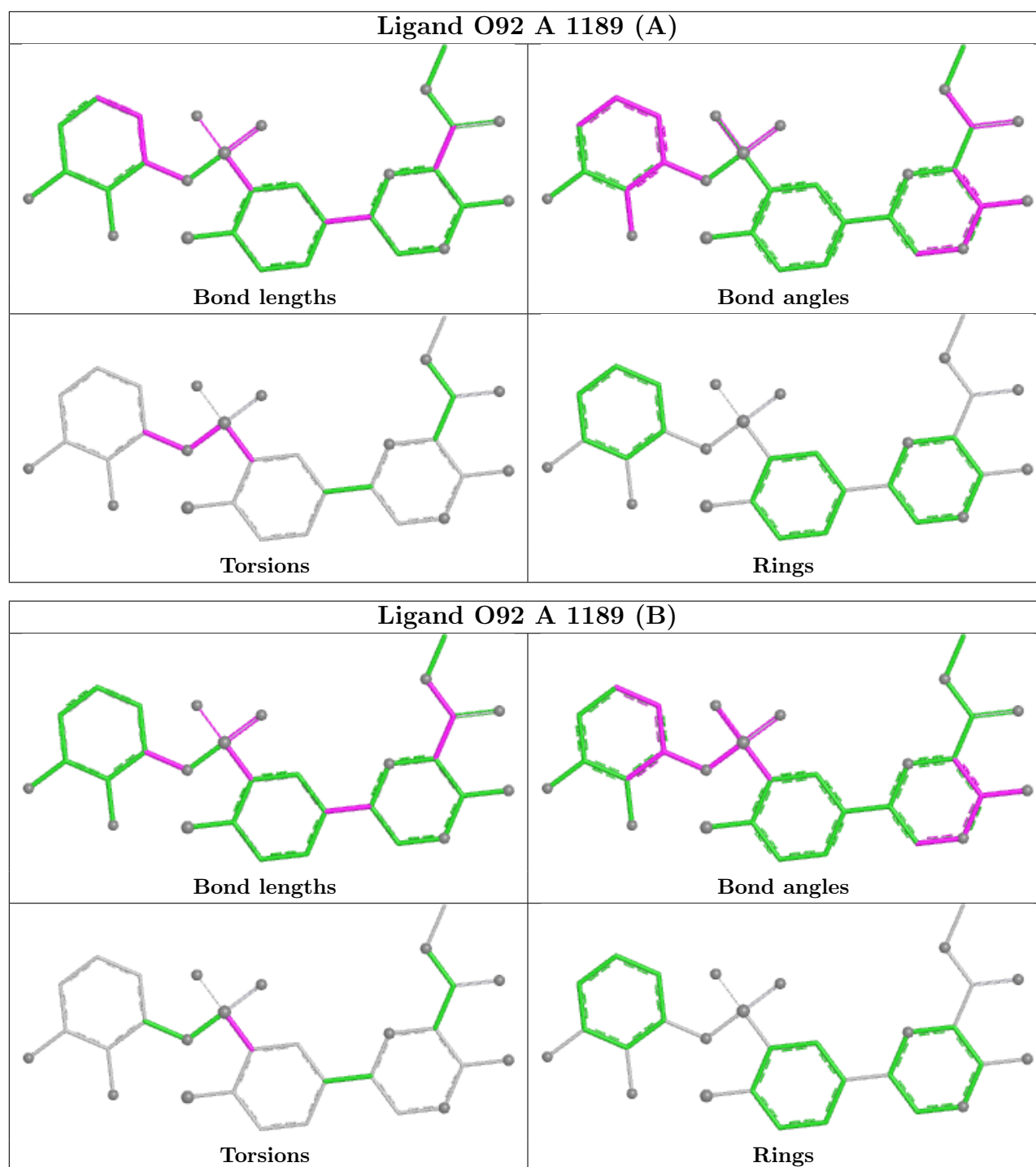
Mol	Chain	Res	Type	Atoms
3	A	1189[A]	O92	C17-C14-N5-S1
3	A	1189[A]	O92	C13-C14-N5-S1
3	A	1189[B]	O92	C9-C10-S1-N5
3	A	1189[B]	O92	C11-C10-S1-N5
3	A	1189[A]	O92	C11-C10-S1-N5
3	A	1189[A]	O92	C14-N5-S1-O3
3	A	1189[A]	O92	C14-N5-S1-O2
3	A	1189[A]	O92	C14-N5-S1-C10

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1189[A]	O92	4	0
3	A	1189[B]	O92	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 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	833/980 (85%)	1.05	118 (14%) 6 7	36, 65, 102, 115	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	5.2
1	A	379	LEU	5.0
1	A	610	LEU	4.7
1	A	229	THR	4.1
1	A	757	TYR	4.1
1	A	1075	CYS	4.0
1	A	243	ALA	3.9
1	A	923	ALA	3.9
1	A	1046	GLU	3.7
1	A	764	ILE	3.5
1	A	150	PHE	3.5
1	A	968	ILE	3.5
1	A	895	THR	3.4
1	A	546	GLU	3.4
1	A	1087	PHE	3.3
1	A	767	LEU	3.3
1	A	925	VAL	3.3
1	A	240	THR	3.2
1	A	380	THR	3.2
1	A	922	GLN	3.2
1	A	404	PHE	3.2
1	A	179	GLY	3.2
1	A	1040	PRO	3.1
1	A	1069	LEU	3.1
1	A	1043	THR	3.0
1	A	248	PHE	3.0
1	A	909	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	241	PRO	3.0
1	A	497	PHE	2.9
1	A	987	LEU	2.9
1	A	813	LEU	2.8
1	A	898	ASN	2.8
1	A	357	CYS	2.7
1	A	149	ALA	2.7
1	A	210	TYR	2.7
1	A	908	ASN	2.7
1	A	1085	ASN	2.7
1	A	435	CYS	2.7
1	A	1064	ALA	2.7
1	A	899	THR	2.7
1	A	1004	PRO	2.7
1	A	154	LEU	2.7
1	A	897	GLY	2.6
1	A	216	ALA	2.6
1	A	993	PHE	2.6
1	A	896	VAL	2.6
1	A	1074	VAL	2.6
1	A	811	LEU	2.6
1	A	192	ASP	2.6
1	A	381	VAL	2.6
1	A	224	ILE	2.6
1	A	1086	TRP	2.5
1	A	223	VAL	2.5
1	A	306	VAL	2.5
1	A	220	ILE	2.5
1	A	233	ILE	2.5
1	A	395	CYS	2.5
1	A	489	GLY	2.5
1	A	315	LEU	2.5
1	A	287	ILE	2.5
1	A	860	LEU	2.5
1	A	378	ASP	2.5
1	A	153	GLN	2.5
1	A	403	PRO	2.5
1	A	983	VAL	2.4
1	A	948	HIS	2.4
1	A	998	SER	2.4
1	A	1039	MET	2.4
1	A	921	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	2.4
1	A	771	LEU	2.4
1	A	577	HIS	2.4
1	A	726	THR	2.4
1	A	1068	PHE	2.4
1	A	212	TRP	2.4
1	A	780	PRO	2.3
1	A	1042	LEU	2.3
1	A	303	ILE	2.3
1	A	516	ILE	2.3
1	A	249	PHE	2.3
1	A	318	VAL	2.3
1	A	1056	THR	2.3
1	A	902	PHE	2.3
1	A	311	PRO	2.3
1	A	462	TYR	2.3
1	A	211	LEU	2.2
1	A	316	ASP	2.2
1	A	967	HIS	2.2
1	A	831	ILE	2.2
1	A	218	ASN	2.2
1	A	916	PRO	2.2
1	A	988	THR	2.2
1	A	373	LEU	2.2
1	A	992	LEU	2.2
1	A	759	VAL	2.2
1	A	1006	PHE	2.2
1	A	1079	GLY	2.2
1	A	487	ILE	2.2
1	A	865	LEU	2.2
1	A	862	LEU	2.1
1	A	994	VAL	2.1
1	A	991	PHE	2.1
1	A	219	CYS	2.1
1	A	147	SER	2.1
1	A	232	THR	2.1
1	A	746	THR	2.1
1	A	522	ASN	2.1
1	A	926	GLU	2.1
1	A	887	THR	2.1
1	A	770	LYS	2.1
1	A	752	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	754	ALA	2.1
1	A	313	PRO	2.1
1	A	244	ILE	2.0
1	A	821	THR	2.0
1	A	1002	THR	2.0
1	A	550	GLN	2.0
1	A	989	PRO	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](#)

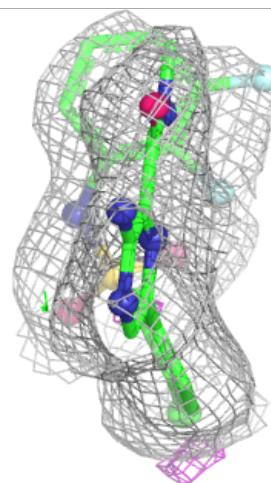
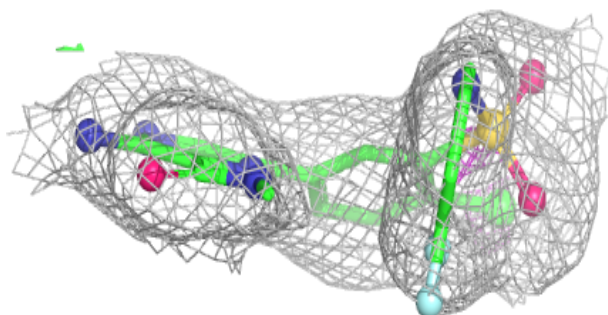
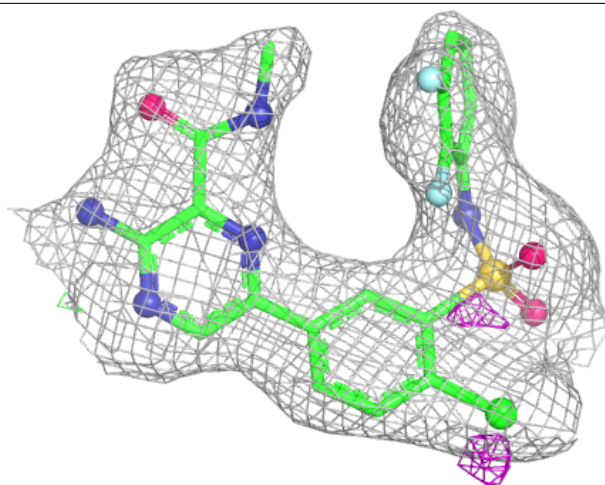
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

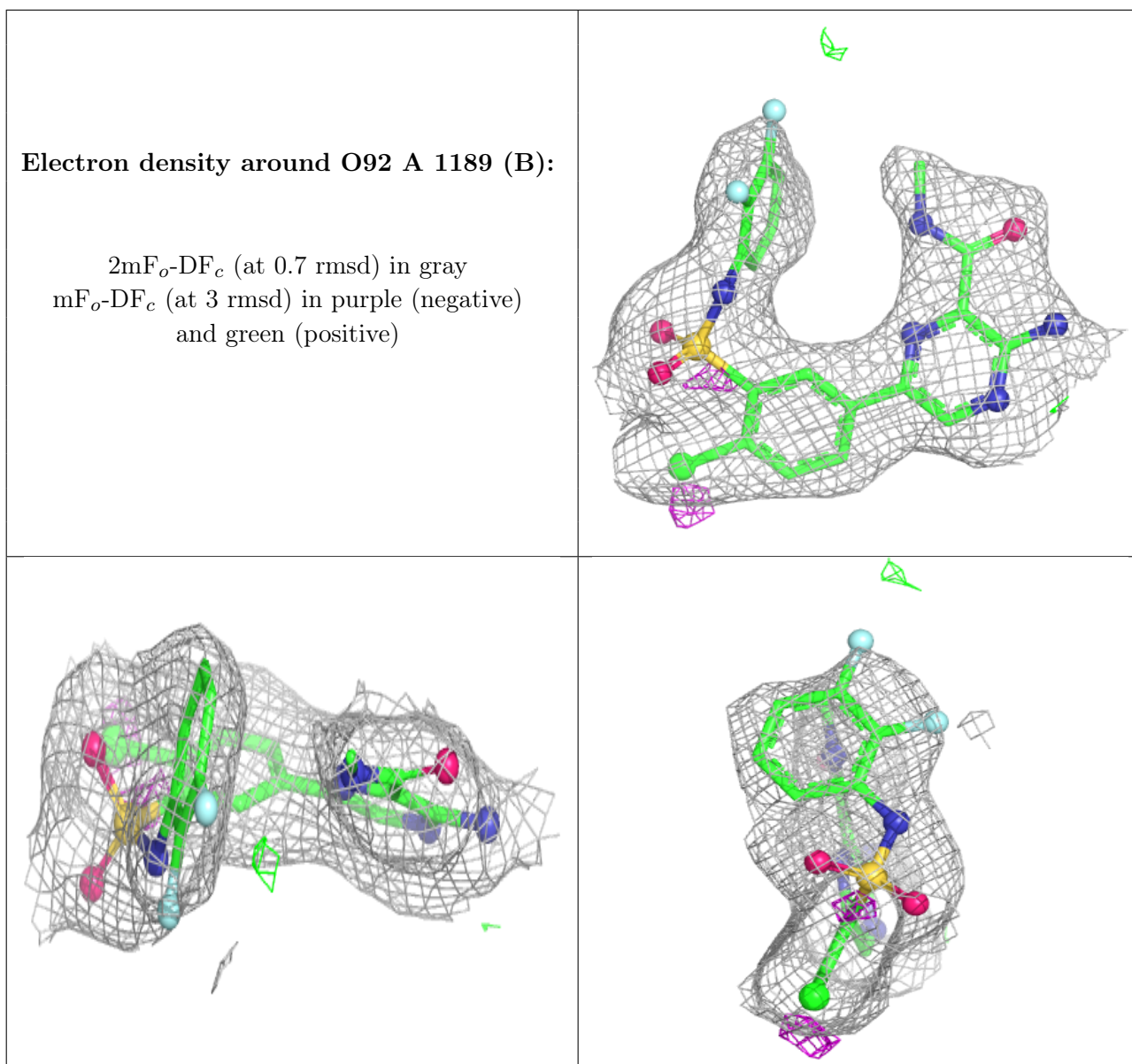
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	1188	5/5	0.89	0.09	75,76,79,81	0
3	O92	A	1189[A]	30/30	0.91	0.11	54,59,74,75	30
3	O92	A	1189[B]	30/30	0.91	0.11	50,57,71,71	30

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 O92 A 1189 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.