



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:37 AM UTC

PDB ID : 4CFW / pdb_00004cfw
Title : Structure-based design of C8-substituted O6-cyclohexylmethoxyguanine
CDK1 and 2 inhibitors.
Authors : Carbain, B.; Paterson, D.J.; Anscombe, E.; Campbell, A.; Cano, C.; Echalié,
A.; Endicott, J.; Golding, B.T.; Haggerty, K.; Hardcastle, I.R.; Jewsbury, P.;
Newell, D.R.; Noble, M.E.M.; Roche, C.; Wang, L.Z.; Griffin, R.
Deposited on : 2013-11-19
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

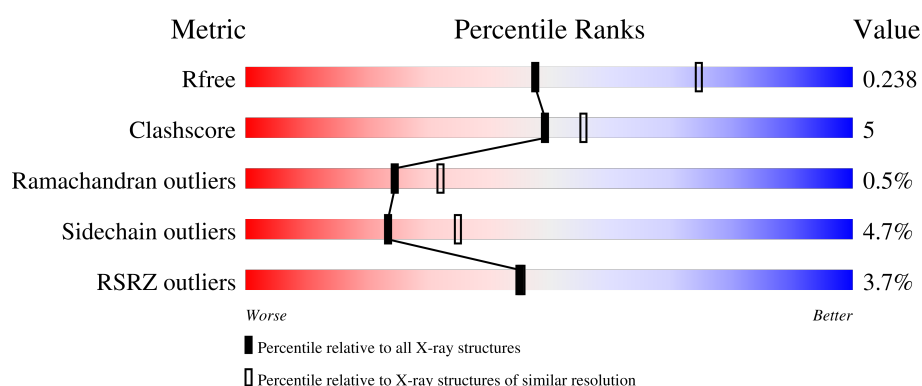
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	6% 79% 18% ..
1	C	303	2% 83% 14% ..
2	B	258	2% 89% 9% .
2	D	258	3% 91% 7% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9736 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 CYCLIN-DEPENDENT KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	P	S	0	7	0
			2458	1590	418	440	1	9			
1	C	298	Total	C	N	O	P	S	0	6	0
			2431	1572	412	437	1	9			

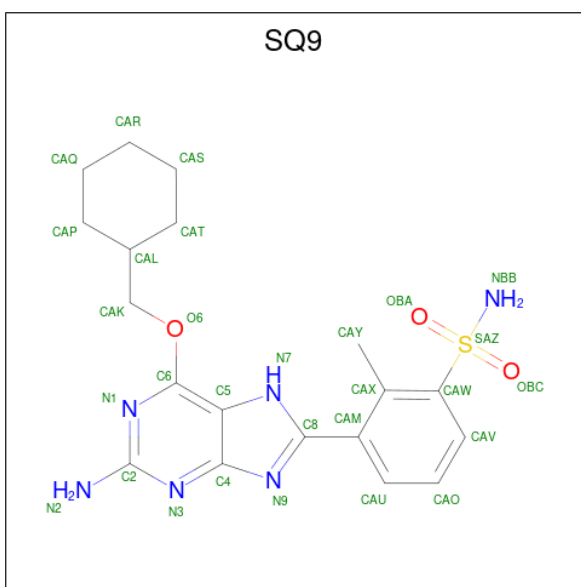
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-4	GLY	-	expression tag	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	LEU	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	8	0
			2140	1384	348	394	14			
2	D	257	Total	C	N	O	S	0	7	0
			2125	1373	345	393	14			

- Molecule 3 is 3-[2-amino-6-(cyclohexylmethoxy)-7H-purin-8-yl]-2-methylbenzenesulfonamide (CCD ID: SQ9) (formula: C₁₉H₂₄N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			29	19	6	3	1		
3	C	1	Total	C	N	O	S	0	0
			29	19	6	3	1		

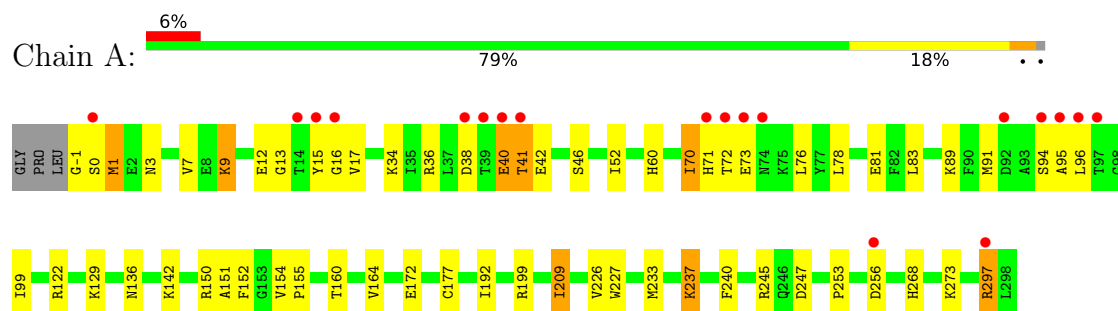
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	188	Total	O	0	0
			188	188		
4	B	151	Total	O	0	0
			151	151		
4	C	108	Total	O	0	0
			108	108		
4	D	77	Total	O	0	0
			77	77		

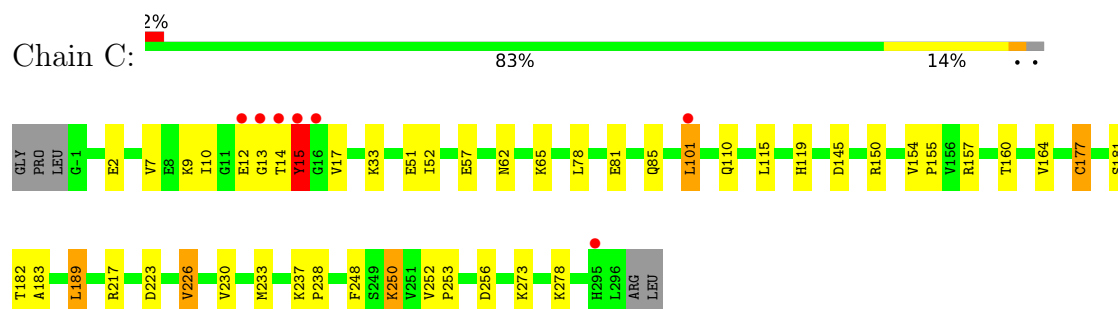
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

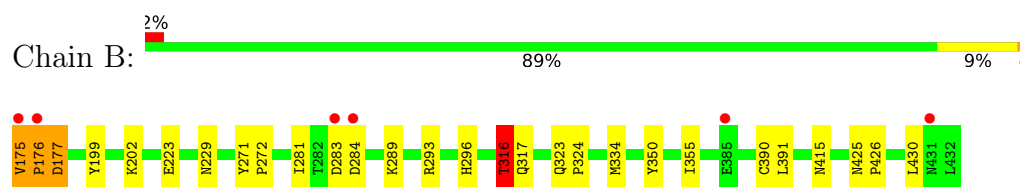
• Molecule 1: CYCLIN-DEPENDENT KINASE 2



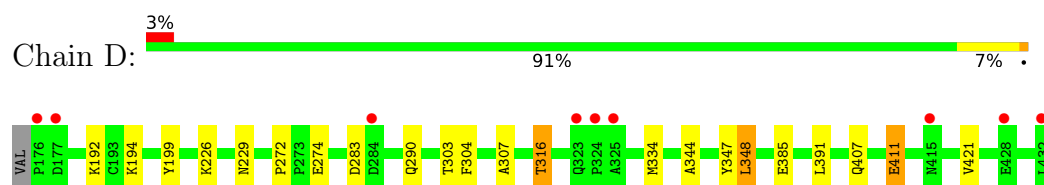
• Molecule 1: CYCLIN-DEPENDENT KINASE 2



• Molecule 2: CYCLIN-A2



• Molecule 2: CYCLIN-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.19Å 134.83Å 148.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.25 – 2.45 37.25 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.25-2.45) 99.3 (37.25-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.185 , 0.241 0.185 , 0.238	Depositor DCC
R_{free} test set	2766 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9736	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: TPO, SQ9

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	1.16	2/2508 (0.1%)	1.13	9/3402 (0.3%)
1	C	1.01	0/2481	1.08	4/3366 (0.1%)
2	B	1.13	2/2190 (0.1%)	1.10	6/2973 (0.2%)
2	D	1.04	3/2175 (0.1%)	1.06	3/2951 (0.1%)
All	All	1.08	7/9354 (0.1%)	1.09	22/12692 (0.2%)

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	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	272	PRO	CA-C	6.19	1.55	1.51
1	A	151	ALA	C-O	-6.04	1.16	1.23
2	D	290	GLN	C-O	-5.89	1.17	1.24
1	A	256	ASP	CB-CG	5.64	1.66	1.52
2	B	223	GLU	C-O	-5.12	1.18	1.24
2	B	284	ASP	CA-C	5.07	1.59	1.53
2	D	283	ASP	N-CA	5.02	1.54	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	199	TYR	N-CA-C	8.11	121.14	111.33
2	B	316	THR	N-CA-CB	-7.21	99.52	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	GLU	N-CA-C	6.59	124.84	110.80
1	A	12	GLU	N-CA-C	-6.58	99.11	109.50
1	C	85	GLN	N-CA-C	6.58	117.26	108.38
1	A	60	HIS	CA-C-N	-6.41	113.20	119.87
1	A	60	HIS	C-N-CA	-6.41	113.20	119.87
1	A	7	VAL	N-CA-C	-6.16	106.91	111.90
2	B	271	TYR	CA-C-N	-6.14	115.24	119.66
2	B	271	TYR	C-N-CA	-6.14	115.24	119.66
2	D	347	TYR	N-CA-C	5.92	118.69	111.82
1	A	253	PRO	N-CA-C	5.90	117.89	110.70
1	C	7	VAL	N-CA-C	-5.89	106.07	111.67
1	A	38	ASP	N-CA-C	5.46	122.42	110.80
2	B	272	PRO	CA-C-N	-5.30	114.32	119.78
2	B	272	PRO	C-N-CA	-5.30	114.32	119.78
1	C	253	PRO	N-CA-C	5.30	117.16	110.70
1	C	15	TYR	N-CA-C	5.22	116.66	111.07
2	B	223	GLU	CB-CA-C	-5.19	102.73	110.88
2	D	421	VAL	N-CA-C	5.12	117.44	111.05
1	A	245	ARG	CA-C-N	-5.01	113.62	122.74
1	A	245	ARG	C-N-CA	-5.01	113.62	122.74

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ILE	Peptide
1	A	72	THR	Peptide

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	2458	0	2495	44	0
1	C	2431	0	2460	31	0
2	B	2140	0	2158	22	0
2	D	2125	0	2138	11	0
3	A	29	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	29	0	24	2	0
4	A	188	0	0	8	1
4	B	151	0	0	3	0
4	C	108	0	0	3	0
4	D	77	0	0	0	1
All	All	9736	0	9297	100	1

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 5.

All (100) 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:C:177[A]:CYS:SG	1:C:233:MET:SD	2.37	1.22
2:B:175:VAL:O	2:B:177:ASP:N	1.81	1.11
2:B:415:ASN:HB3	4:B:2144:HOH:O	1.48	1.07
1:A:95:ALA:O	1:A:96:LEU:HB2	1.67	0.90
1:A:297:ARG:HH11	1:A:297:ARG:HG3	1.34	0.88
2:B:175:VAL:C	2:B:177:ASP:H	1.83	0.86
1:A:237:LYS:HE2	4:A:2141:HOH:O	1.72	0.86
2:B:350:TYR:HB2	2:B:355[B]:ILE:HD11	1.60	0.83
1:C:154:VAL:O	2:D:316:THR:CG2	2.26	0.83
1:A:15:TYR:HD1	1:A:16:GLY:H	1.27	0.83
2:B:175:VAL:HG12	2:B:177:ASP:HB2	1.63	0.81
1:A:9:LYS:HD3	1:A:17:VAL:CG1	2.10	0.80
1:C:154:VAL:O	2:D:316:THR:HG22	1.82	0.79
1:A:-1:GLY:N	4:A:2001:HOH:O	2.07	0.78
1:C:81:GLU:O	3:C:1297:SQ9:N2	2.16	0.78
1:A:42:GLU:OE2	4:A:2025:HOH:O	2.05	0.73
2:B:350:TYR:CB	2:B:355[B]:ILE:HD11	2.18	0.73
1:A:13:GLY:HA3	1:A:15:TYR:CE1	2.25	0.72
1:A:209:ILE:HG12	4:A:2123:HOH:O	1.89	0.71
1:A:297:ARG:HG3	1:A:297:ARG:NH1	2.05	0.69
1:C:51:GLU:OE2	4:C:2023:HOH:O	2.11	0.69
1:A:3:ASN:HB2	4:A:2001:HOH:O	1.94	0.67
4:A:2031:HOH:O	2:B:316:THR:HG21	1.93	0.67
1:A:154:VAL:O	2:B:316:THR:HG23	1.96	0.64
1:A:154:VAL:O	2:B:316:THR:CG2	2.47	0.63
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.79	0.63
1:C:15:TYR:CD2	1:C:33:LYS:HE3	2.33	0.63
1:A:1:MET:HG2	1:A:70:ILE:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:HA	1:A:76:LEU:HD12	1.80	0.62
1:A:0:SER:O	1:A:1:MET:HB2	2.01	0.60
1:A:297:ARG:HH11	1:A:297:ARG:CG	2.10	0.60
2:B:415:ASN:ND2	4:B:2143:HOH:O	2.35	0.59
1:C:13:GLY:HA3	1:C:15:TYR:CZ	2.37	0.59
4:C:2063:HOH:O	2:D:316:THR:HG21	2.03	0.58
2:B:175:VAL:C	2:B:177:ASP:N	2.50	0.58
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.85	0.57
1:C:101:LEU:HD22	1:C:101:LEU:H	1.70	0.57
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.40	0.56
1:A:9:LYS:HD3	1:A:17:VAL:HG12	1.88	0.55
2:B:355[B]:ILE:HD13	2:B:355[B]:ILE:N	2.20	0.55
1:A:177[A]:CYS:SG	1:A:233:MET:SD	3.06	0.53
2:D:303:THR:O	2:D:304:PHE:HB2	2.09	0.53
2:D:407:GLN:O	2:D:411:GLU:HG2	2.09	0.52
1:A:0:SER:O	1:A:1:MET:CB	2.57	0.52
1:A:83:LEU:HD21	1:A:142:LYS:HE3	1.93	0.51
2:D:229:ASN:HD22	2:D:334[B]:MET:HE3	1.76	0.51
1:C:181:SER:O	1:C:183:ALA:N	2.44	0.50
2:D:229:ASN:HD22	2:D:334[A]:MET:HE2	1.77	0.50
1:A:15:TYR:HD1	1:A:16:GLY:N	2.05	0.50
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.93	0.50
2:B:317:GLN:NE2	4:B:2018:HOH:O	2.20	0.50
1:A:81:GLU:O	3:A:1299:SQ9:N2	2.42	0.50
1:A:94:SER:HA	4:A:2056:HOH:O	2.12	0.49
2:B:293:ARG:NH2	1:C:2:GLU:HG2	2.27	0.49
1:A:40:GLU:OE1	1:A:41:THR:N	2.47	0.48
1:C:230:VAL:HA	1:C:233:MET:CE	2.43	0.48
1:A:268:HIS:CD2	4:A:2134:HOH:O	2.66	0.48
1:C:15:TYR:CD1	1:C:15:TYR:N	2.70	0.48
1:C:115:LEU:HD22	1:C:189:LEU:HD22	1.96	0.48
1:C:119:HIS:CE1	1:C:182:THR:HB	2.48	0.48
2:B:229:ASN:HD22	2:B:334[A]:MET:HE2	1.79	0.47
1:C:145:ASP:HB2	3:C:1297:SQ9:HAT	1.96	0.47
2:D:344:ALA:O	2:D:348[A]:LEU:HB2	2.15	0.46
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.51	0.46
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.30	0.46
1:A:172:GLU:O	1:A:177[B]:CYS:SG	2.75	0.45
2:B:175:VAL:O	2:B:176:PRO:C	2.53	0.45
1:C:273:LYS:HD3	1:C:273:LYS:HA	1.81	0.45
1:C:250:LYS:HD2	1:C:250:LYS:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:VAL:O	1:C:233:MET:CG	2.66	0.44
1:C:230:VAL:O	1:C:233:MET:HG2	2.18	0.44
2:B:199:TYR:C	2:B:199:TYR:CD1	2.95	0.43
1:C:230:VAL:HA	1:C:233:MET:HE2	2.00	0.43
1:A:237:LYS:HZ2	1:A:240:PHE:HE1	1.59	0.43
1:C:256:ASP:OD1	1:C:256:ASP:N	2.49	0.43
1:A:9:LYS:HD3	1:A:17:VAL:HG13	1.95	0.43
2:B:355[B]:ILE:HD12	2:B:390:CYS:SG	2.58	0.43
1:A:155:PRO:HD2	2:B:316:THR:HG23	2.01	0.43
1:C:52:ILE:HD11	1:C:78:LEU:HD21	2.00	0.43
2:B:430:LEU:HA	2:B:430:LEU:HD23	1.76	0.42
1:C:181:SER:O	1:C:182:THR:C	2.61	0.42
1:C:223:ASP:OD1	1:C:226:VAL:HG13	2.19	0.42
2:D:229:ASN:ND2	2:D:334[A]:MET:HE2	2.34	0.42
1:A:83:LEU:HD23	1:A:136:ASN:HB3	2.01	0.42
1:A:13:GLY:C	1:A:15:TYR:H	2.28	0.42
1:A:237:LYS:NZ	1:A:237:LYS:HB2	2.35	0.42
1:A:15:TYR:CD1	1:A:16:GLY:N	2.81	0.41
1:A:83:LEU:O	3:A:1299:SQ9:N9	2.54	0.41
2:B:323:GLN:HA	2:B:324:PRO:HA	1.87	0.41
1:C:217:ARG:NH1	4:C:2092:HOH:O	2.47	0.41
1:A:129:LYS:HA	1:A:192:ILE:HD11	2.02	0.41
1:A:199:ARG:CZ	1:A:199:ARG:HB2	2.50	0.41
1:A:227:TRP:CZ2	1:A:233:MET:HE1	2.56	0.41
2:B:425:ASN:HA	2:B:426:PRO:HD3	1.98	0.41
1:C:101:LEU:HD13	1:C:101:LEU:N	2.36	0.40
1:A:16:GLY:HA3	1:A:34:LYS:O	2.21	0.40
1:C:57:GLU:OE2	2:D:307:ALA:HB3	2.20	0.40
1:A:71:HIS:CG	1:A:71:HIS:O	2.74	0.40
1:C:237:LYS:HA	1:C:238:PRO:HD2	1.94	0.40
1:C:189:LEU:HA	1:C:189:LEU:HD12	1.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2049:HOH:O	4:D:2076:HOH:O[1_655]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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	304/303 (100%)	291 (96%)	11 (4%)	2 (1%)	18	24
1	C	301/303 (99%)	292 (97%)	6 (2%)	3 (1%)	12	14
2	B	264/258 (102%)	260 (98%)	3 (1%)	1 (0%)	30	37
2	D	262/258 (102%)	259 (99%)	3 (1%)	0	100	100
All	All	1131/1122 (101%)	1102 (97%)	23 (2%)	6 (0%)	24	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	176	PRO
1	A	164	VAL
1	C	164	VAL
1	A	1	MET
1	C	177[A]	CYS
1	C	177[B]	CYS

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	270/265 (102%)	257 (95%)	13 (5%)	23	34
1	C	267/265 (101%)	251 (94%)	16 (6%)	17	26
2	B	240/232 (103%)	230 (96%)	10 (4%)	26	39
2	D	238/232 (103%)	228 (96%)	10 (4%)	26	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1015/994 (102%)	966 (95%)	49 (5%)	23	34

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	36	ARG
1	A	40	GLU
1	A	41	THR
1	A	46[A]	SER
1	A	46[B]	SER
1	A	89	LYS
1	A	150	ARG
1	A	209	ILE
1	A	226	VAL
1	A	237	LYS
1	A	247	ASP
1	A	297	ARG
2	B	175	VAL
2	B	177	ASP
2	B	202	LYS
2	B	281	ILE
2	B	283	ASP
2	B	289	LYS
2	B	296	HIS
2	B	316	THR
2	B	391[A]	LEU
2	B	391[B]	LEU
1	C	9	LYS
1	C	10	ILE
1	C	12	GLU
1	C	14	THR
1	C	15	TYR
1	C	17	VAL
1	C	65	LYS
1	C	101	LEU
1	C	150	ARG
1	C	157	ARG
1	C	189	LEU
1	C	226	VAL
1	C	248	PHE
1	C	250	LYS

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Mol	Chain	Res	Type
1	C	252	VAL
1	C	278	LYS
2	D	192	LYS
2	D	194	LYS
2	D	226	LYS
2	D	274	GLU
2	D	316	THR
2	D	348[A]	LEU
2	D	348[B]	LEU
2	D	385	GLU
2	D	391	LEU
2	D	411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	85	GLN
1	A	287	GLN
2	B	313	GLN
2	B	406	GLN
2	B	419	HIS
1	C	113	GLN
1	C	268	HIS
2	D	370	GLN
2	D	396	GLN
2	D	425	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	160	1	8,10,11	0.91	0	10,14,16	1.08	1 (10%)
1	TPO	C	160	1	8,10,11	0.80	0	10,14,16	1.34	2 (20%)

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
1	TPO	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	0/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	160	TPO	OG1-P-O1P	-2.21	101.47	109.33
1	A	160	TPO	O3P-P-O2P	2.13	115.81	107.80
1	C	160	TPO	O-C-CA	-2.13	119.29	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SQ9	C	1297	-	31,32,32	3.25	13 (41%)	40,47,47	1.83	10 (25%)
3	SQ9	A	1299	-	31,32,32	4.89	10 (32%)	40,47,47	2.40	15 (37%)

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	SQ9	C	1297	-	-	4/15/23/23	0/4/4/4
3	SQ9	A	1299	-	-	7/15/23/23	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1299	SQ9	SAZ-NBB	-21.53	1.18	1.60
3	C	1297	SQ9	SAZ-NBB	-7.78	1.45	1.60
3	C	1297	SQ9	OBA-SAZ	7.77	1.57	1.43
3	C	1297	SQ9	CAM-C8	-7.44	1.34	1.47
3	A	1299	SQ9	CAW-SAZ	6.83	1.86	1.77
3	A	1299	SQ9	OBA-SAZ	6.68	1.55	1.43
3	C	1297	SQ9	OBC-SAZ	6.64	1.55	1.43
3	A	1299	SQ9	CAM-C8	-6.43	1.36	1.47
3	C	1297	SQ9	CAY-CAX	-6.09	1.39	1.51
3	A	1299	SQ9	OBC-SAZ	5.86	1.54	1.43
3	A	1299	SQ9	CAY-CAX	-5.84	1.40	1.51
3	A	1299	SQ9	C4-N9	-5.34	1.29	1.38
3	C	1297	SQ9	C6-N1	3.35	1.37	1.32
3	A	1299	SQ9	C5-C4	-3.05	1.34	1.40
3	C	1297	SQ9	O6-C6	3.02	1.39	1.34
3	C	1297	SQ9	C4-N9	-3.00	1.33	1.38
3	C	1297	SQ9	CAS-CAT	2.99	1.60	1.53
3	C	1297	SQ9	CAR-CAQ	2.72	1.61	1.51
3	A	1299	SQ9	CAP-CAL	2.68	1.60	1.52
3	C	1297	SQ9	CAT-CAL	2.60	1.60	1.52
3	A	1299	SQ9	C2-N1	-2.34	1.31	1.35
3	C	1297	SQ9	C5-C4	-2.03	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1297	SQ9	CAW-SAZ	2.01	1.80	1.77

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1299	SQ9	OBC-SAZ-OBA	-6.59	108.66	118.80
3	A	1299	SQ9	OBC-SAZ-CAW	5.34	115.02	107.26
3	A	1299	SQ9	C4-C5-N7	4.70	108.78	105.28
3	C	1297	SQ9	C4-C5-N7	4.44	108.58	105.28
3	A	1299	SQ9	CAU-CAM-CAX	-4.43	117.57	120.74
3	C	1297	SQ9	OBC-SAZ-OBA	-4.35	112.11	118.80
3	A	1299	SQ9	N2-C2-N3	4.05	123.29	117.22
3	A	1299	SQ9	N3-C2-N1	-3.29	120.43	125.48
3	C	1297	SQ9	C5-C4-N3	-3.16	121.44	124.22
3	C	1297	SQ9	CAW-SAZ-NBB	3.14	113.93	108.28
3	A	1299	SQ9	OBA-SAZ-CAW	3.08	111.74	107.26
3	A	1299	SQ9	CAX-CAM-C8	3.01	126.47	122.38
3	A	1299	SQ9	CAM-C8-N7	2.92	129.69	124.21
3	C	1297	SQ9	N3-C2-N1	-2.87	121.08	125.48
3	A	1299	SQ9	C5-C4-N3	-2.85	121.71	124.22
3	C	1297	SQ9	CAU-CAM-CAX	-2.80	118.74	120.74
3	C	1297	SQ9	CAM-C8-N7	2.72	129.31	124.21
3	A	1299	SQ9	O6-C6-C5	2.52	119.70	115.40
3	C	1297	SQ9	CAV-CAW-SAZ	-2.51	114.11	117.52
3	A	1299	SQ9	OBA-SAZ-NBB	-2.24	104.13	107.35
3	C	1297	SQ9	C2-N1-C6	2.18	119.00	115.96
3	A	1299	SQ9	CAM-C8-N9	-2.17	119.88	123.65
3	C	1297	SQ9	CAM-C8-N9	-2.14	119.93	123.65
3	A	1299	SQ9	C2-N1-C6	2.10	118.88	115.96
3	A	1299	SQ9	C5-C4-N9	-2.01	108.68	110.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1299	SQ9	N1-C6-O6-CAK
3	A	1299	SQ9	C5-C6-O6-CAK
3	A	1299	SQ9	CAL-CAK-O6-C6
3	A	1299	SQ9	O6-CAK-CAL-CAT
3	C	1297	SQ9	N1-C6-O6-CAK
3	C	1297	SQ9	C5-C6-O6-CAK
3	A	1299	SQ9	O6-CAK-CAL-CAP

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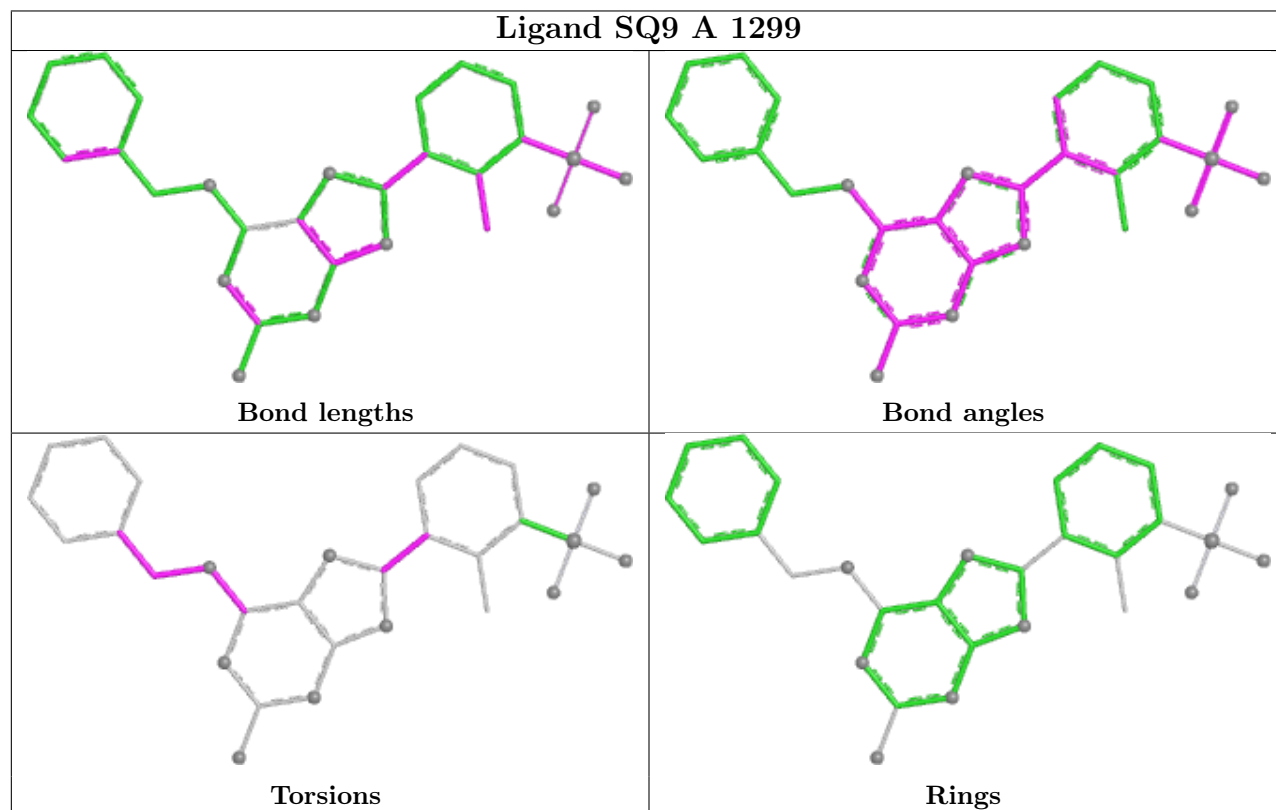
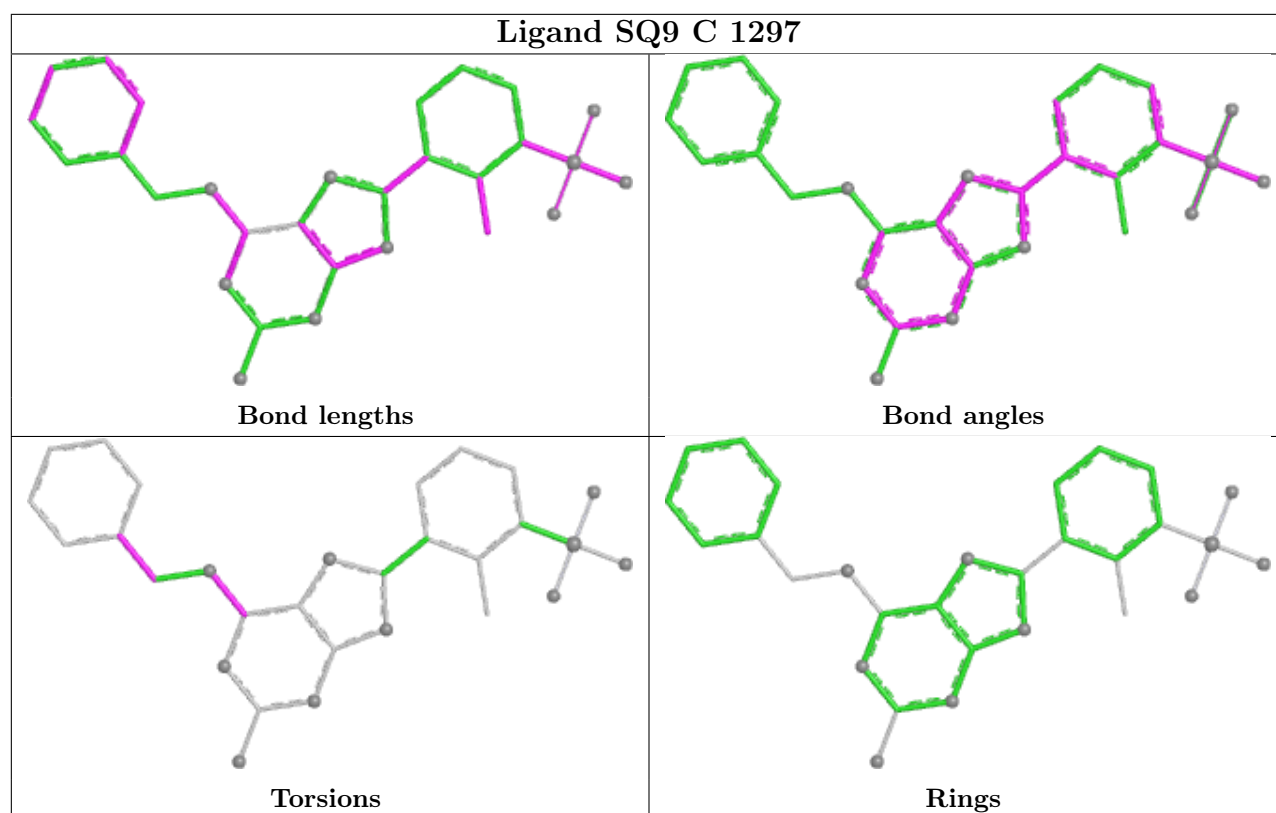
Mol	Chain	Res	Type	Atoms
3	A	1299	SQ9	N9-C8-CAM-CAX
3	A	1299	SQ9	N9-C8-CAM-CAU
3	C	1297	SQ9	O6-CAK-CAL-CAP
3	C	1297	SQ9	O6-CAK-CAL-CAT

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	SQ9	2	0
3	A	1299	SQ9	2	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(Å²)	Q<0.9	
1	A	299/303 (98%)	-0.17	19 (6%)	25	23	9, 26, 52, 70	7 (2%)
1	C	297/303 (98%)	-0.10	7 (2%)	59	62	15, 38, 53, 63	6 (2%)
2	B	258/258 (100%)	-0.37	6 (2%)	61	63	10, 28, 44, 57	8 (3%)
2	D	257/258 (99%)	-0.04	9 (3%)	47	47	16, 39, 65, 82	7 (2%)
All	All	1111/1122 (99%)	-0.17	41 (3%)	45	45	9, 33, 57, 82	28 (2%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	TYR	5.3
1	A	41	THR	4.7
1	C	14	THR	4.6
2	B	176	PRO	4.5
2	D	176	PRO	4.3
1	A	15	TYR	4.0
2	B	175	VAL	4.0
2	B	284	ASP	3.9
2	D	177	ASP	3.5
1	A	39	THR	3.5
2	D	323	GLN	3.4
1	A	73	GLU	3.4
1	A	14	THR	3.3
1	A	96	LEU	3.3
1	A	95	ALA	3.1
2	B	283	ASP	3.1
2	D	432	LEU	3.1
1	A	40	GLU	2.9
1	A	0	SER	2.9
1	C	13	GLY	2.7
1	A	297	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	385	GLU	2.7
1	A	74	ASN	2.6
2	B	431	ASN	2.5
1	C	295	HIS	2.5
1	A	256	ASP	2.5
2	D	284	ASP	2.5
1	A	72	THR	2.5
1	C	12	GLU	2.4
1	A	97	THR	2.4
1	A	94	SER	2.4
2	D	428[A]	GLU	2.4
1	C	16	GLY	2.4
1	A	38	ASP	2.4
2	D	324	PRO	2.3
1	A	16	GLY	2.3
1	A	71	HIS	2.2
1	C	101	LEU	2.2
2	D	325	ALA	2.1
2	D	415	ASN	2.1
1	A	92	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	C	160	11/12	0.98	0.06	30,33,34,34	0
1	TPO	A	160	11/12	0.99	0.05	23,25,26,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

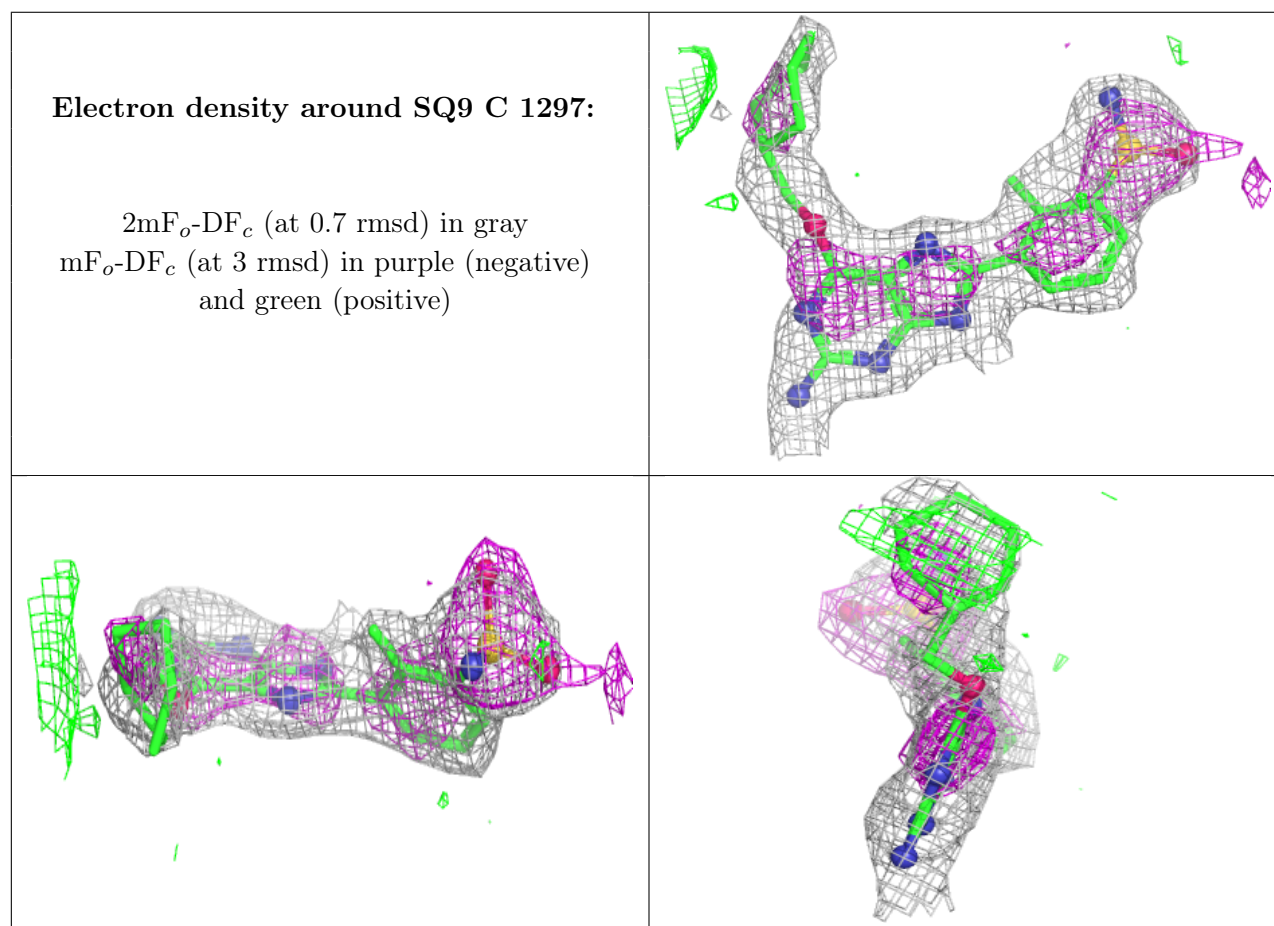
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

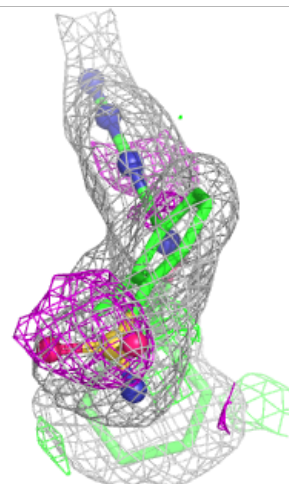
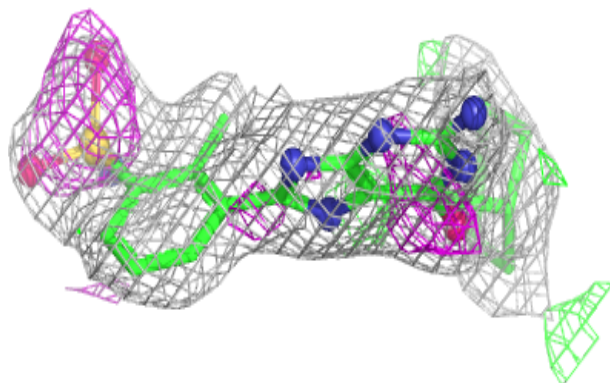
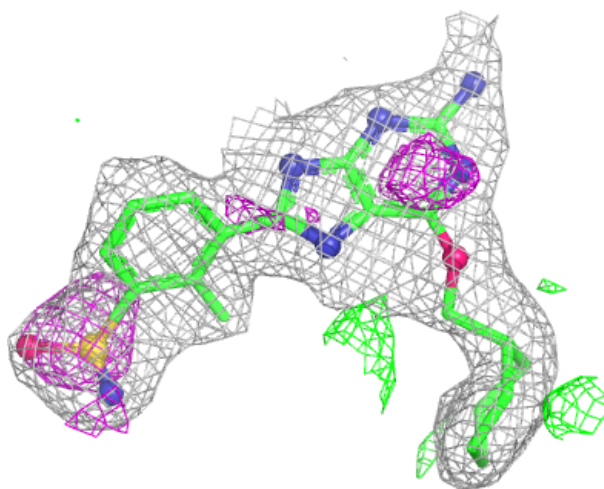
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SQ9	C	1297	29/29	0.82	0.15	39,43,50,51	0
3	SQ9	A	1299	29/29	0.86	0.13	35,39,44,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around SQ9 A 1299:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.