



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:30 PM UTC

PDB ID : 2IW9 / pdb_00002iw9
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2-CYCLIN A COM-
PLEXED WITH A BISANILINOPYRIMIDINE INHIBITOR
Authors : Pratt, D.J.; Bentley, J.; Jewsbury, P.; Boyle, F.T.; Endicott, J.A.; Noble,
M.E.M.
Deposited on : 2006-06-27
Resolution : 2.00 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

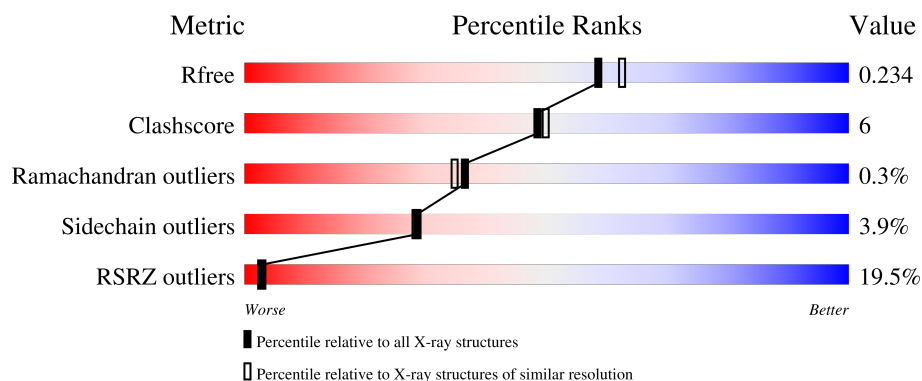
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	302	
1	C	302	
2	B	260	
2	D	260	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9155 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	P	S	0	5	0
			2391	1552	409	421	1	8			
1	C	269	Total	C	N	O	P	S	0	3	0
			2166	1405	368	385	1	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
A	89	THR	LYS	engineered mutation	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941
C	89	THR	LYS	engineered mutation	UNP P24941

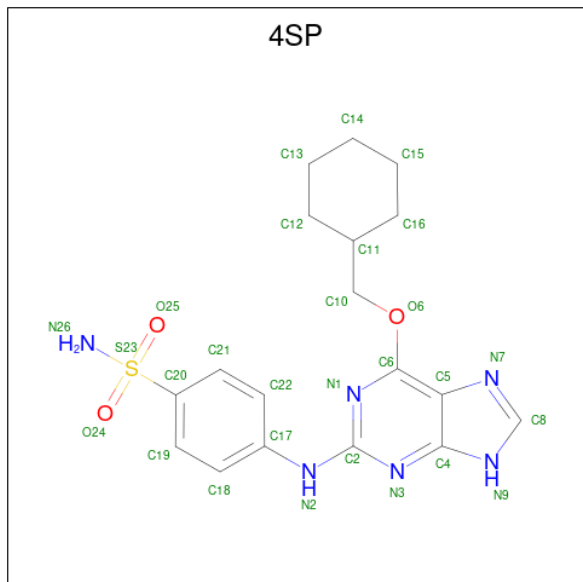
- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S	0	4	0
			2076	1347	336	381	12			
2	D	255	Total	C	N	O	S	0	1	0
			2068	1340	339	378	11			

There are 2 discrepancies between the modelled and reference sequences:

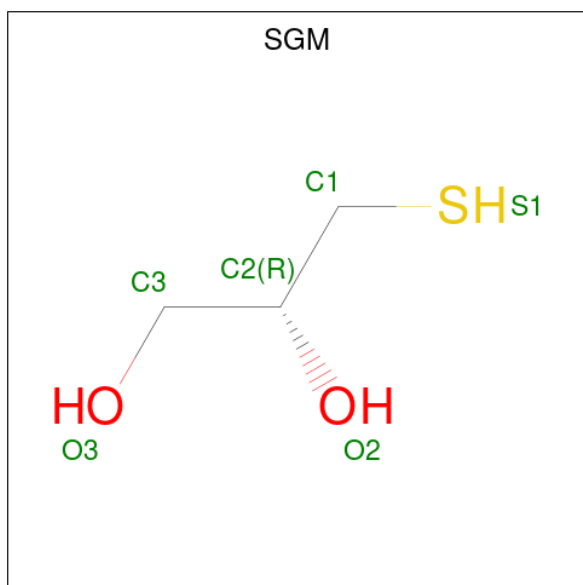
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	expression tag	UNP P20248
D	173	MET	-	expression tag	UNP P20248

- Molecule 3 is O6-CYCLOHEXYLMETHOXY-2-(4'-SULPHAMOYLANILINO) PURINE (CCD ID: 4SP) (formula: $C_{18}H_{22}N_6O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	18	6	3	1		
3	C	1	Total	C	N	O	S	0	0
			28	18	6	3	1		

- Molecule 4 is MONOTHIOGLYCEROL (CCD ID: SGM) (formula: $C_3H_8O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			6	3	2	1		
4	D	1	Total	C	O	S	0	0
			6	3	2	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

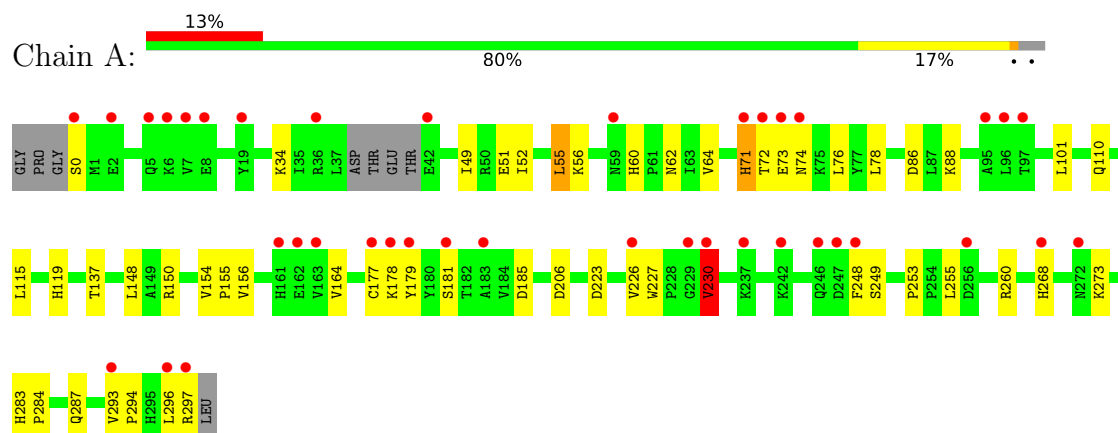
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total	O	0	0
			171	171		
6	B	122	Total	O	0	0
			122	122		
6	C	49	Total	O	0	0
			49	49		
6	D	42	Total	O	0	0
			42	42		

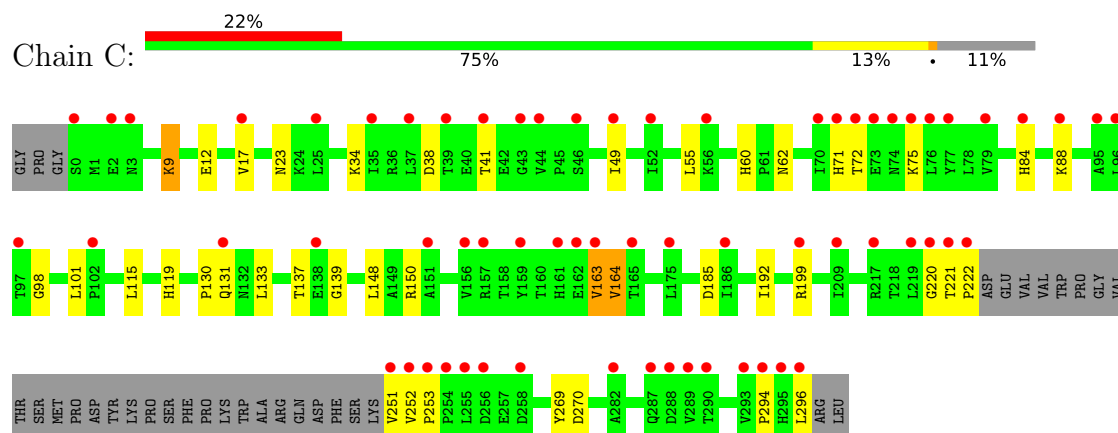
3 Residue-property plots [i](#)

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.

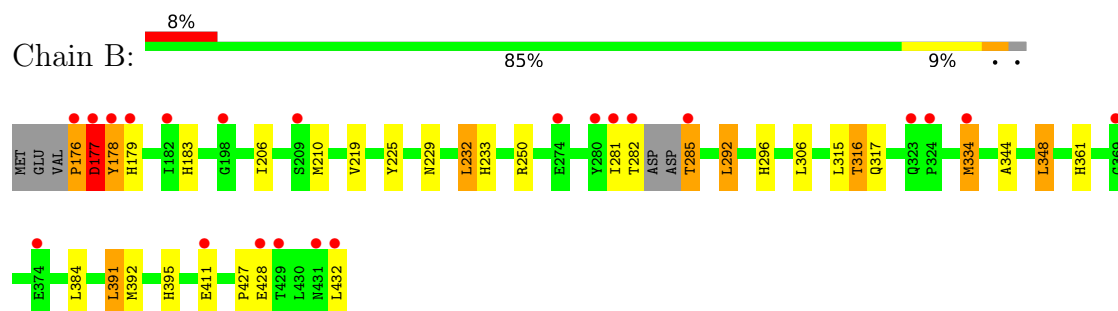
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



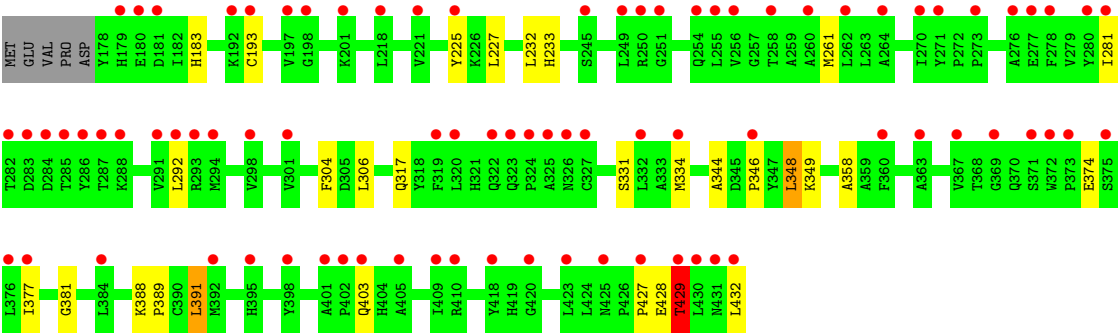
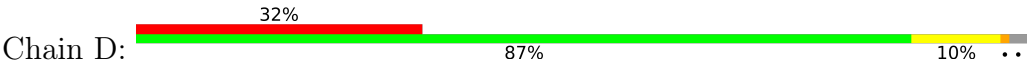
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• 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	73.76Å 134.10Å 148.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.00 99.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (100.00-2.00) 97.6 (99.41-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.240 0.206 , 0.234	Depositor DCC
R_{free} test set	4861 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9155	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: MG, 4SP, TPO, SGM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	0/2462	0.89	2/3339 (0.1%)
1	C	0.57	0/2217	0.84	3/3006 (0.1%)
2	B	0.69	0/2141	0.88	1/2903 (0.0%)
2	D	0.91	8/2121 (0.4%)	0.89	1/2878 (0.0%)
All	All	0.73	8/8941 (0.1%)	0.88	7/12126 (0.1%)

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
2	B	0	2
2	D	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	429	THR	C-O	18.15	1.48	1.23
2	D	429	THR	C-N	12.85	1.53	1.33
2	D	374	GLU	CD-OE1	10.80	1.45	1.25
2	D	374	GLU	CD-OE2	10.65	1.45	1.25
2	D	403	GLN	CD-OE1	8.02	1.38	1.23
2	D	428	GLU	C-O	7.76	1.33	1.24
2	D	381	GLY	C-O	6.45	1.33	1.24
2	D	377	ILE	C-N	6.39	1.42	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CB-CA-C	-8.99	100.01	112.14
1	C	253	PRO	N-CA-C	6.49	118.61	110.70
2	B	178	TYR	N-CA-C	-5.68	106.73	113.38
1	A	253	PRO	N-CA-C	5.55	117.47	110.70
2	D	374	GLU	OE1-CD-OE2	5.12	135.18	122.90
1	C	270	ASP	CA-C-N	5.07	125.10	119.32
1	C	270	ASP	C-N-CA	5.07	125.10	119.32

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	176	PRO	Peptide
2	B	177	ASP	Peptide
2	D	429	THR	Mainchain

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	2391	0	2424	38	0
1	C	2166	0	2217	25	0
2	B	2076	0	2099	29	0
2	D	2068	0	2096	13	0
3	A	28	0	22	2	0
3	C	28	0	22	1	0
4	B	6	0	7	0	0
4	D	6	0	8	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	171	0	0	3	0
6	B	122	0	0	4	0
6	C	49	0	0	1	0
6	D	42	0	0	2	0
All	All	9155	0	8895	98	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 6.

All (98) 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)
2:D:193:CYS:SG	4:D:1433:SGM:S1	2.54	0.91
1:A:154:VAL:O	2:B:316:THR:HG22	1.75	0.86
1:A:137:THR:O	1:A:293:VAL:HG13	1.80	0.82
1:A:227:TRP:O	1:A:230:VAL:HG22	1.85	0.77
1:A:268[B]:HIS:CD2	1:A:273:LYS:HB2	2.21	0.76
2:D:331:SER:HA	2:D:334:MET:HE2	1.69	0.74
1:A:71[B]:HIS:CD2	2:B:296:HIS:HE1	2.06	0.73
1:A:71[B]:HIS:CD2	2:B:296:HIS:CE1	2.77	0.73
1:A:60:HIS:HD2	1:A:62:ASN:H	1.38	0.71
1:A:60:HIS:CD2	1:A:62:ASN:H	2.11	0.68
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.76	0.68
1:A:296:LEU:O	1:A:297:ARG:HB2	1.92	0.67
1:A:64:VAL:HG21	3:A:1298:4SP:C8	2.25	0.67
1:C:220:GLY:O	1:C:269:TYR:OH	2.08	0.66
1:C:23:ASN:HB2	6:C:2009:HOH:O	1.95	0.66
2:B:395:HIS:HE1	2:B:427:PRO:O	1.80	0.65
1:A:181:SER:OG	6:A:2103:HOH:O	2.14	0.64
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.80	0.62
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.64	0.61
2:B:233:HIS:HE1	6:B:2078:HOH:O	1.83	0.61
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.83	0.60
2:B:315:LEU:HD12	2:B:334[A]:MET:HE3	1.84	0.60
2:B:177:ASP:C	2:B:179:HIS:N	2.60	0.59
2:B:229:ASN:HD22	2:B:334[B]:MET:HE2	1.68	0.59
1:C:60:HIS:HD2	1:C:62:ASN:H	1.51	0.58
1:C:60:HIS:CD2	1:C:62:ASN:H	2.22	0.57
1:A:268[B]:HIS:CD2	6:A:2124:HOH:O	2.56	0.57
2:D:225:TYR:HE1	2:D:281:ILE:HG21	1.70	0.57
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.40	0.57
1:A:284:PRO:O	1:A:287:GLN:HG2	2.05	0.56
1:A:154:VAL:O	2:B:316:THR:CG2	2.51	0.56
1:A:64:VAL:HG21	3:A:1298:4SP:H8	1.85	0.56
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.88	0.55
2:D:346:PRO:O	2:D:349:LYS:HG2	2.06	0.55
2:B:177:ASP:C	2:B:179:HIS:H	2.15	0.54
1:C:88:LYS:HG3	1:C:131:GLN:HE21	1.72	0.54
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.45	0.52
1:C:34:LYS:HE3	1:C:75:LYS:HE3	1.91	0.52
2:D:358:ALA:HA	2:D:391:LEU:HD22	1.93	0.51
1:A:60:HIS:HE1	6:A:2025:HOH:O	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:PRO:O	2:B:177:ASP:HB3	2.11	0.51
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.93	0.51
2:B:392:MET:HE3	2:B:432:LEU:HD12	1.93	0.51
1:A:119:HIS:HD2	6:B:2013:HOH:O	1.93	0.51
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.92	0.50
1:C:71[B]:HIS:CE1	2:D:304:PHE:HE2	2.29	0.50
1:A:137:THR:O	1:A:293:VAL:CG1	2.54	0.50
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.96	0.49
1:A:86:ASP:OD1	1:A:88:LYS:HB3	2.13	0.48
2:B:210:MET:HE1	2:B:250:ARG:CB	2.43	0.48
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.95	0.48
1:C:133:LEU:HD11	1:C:192:ILE:HD13	1.94	0.48
1:A:178:LYS:HE2	1:A:179:TYR:CZ	2.49	0.48
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.96	0.48
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.95	0.48
2:D:233:HIS:HE1	6:D:2037:HOH:O	1.95	0.48
1:C:9:LYS:HE3	1:C:17:VAL:HG13	1.95	0.48
2:B:315:LEU:CD1	2:B:334[A]:MET:HE3	2.43	0.47
1:A:71[B]:HIS:CD2	1:A:76:LEU:HD13	2.50	0.47
1:C:222:PRO:HB3	1:C:269:TYR:CG	2.49	0.47
1:C:88:LYS:HG3	1:C:131:GLN:NE2	2.29	0.47
1:C:115:LEU:HD21	1:C:185:ASP:HB3	1.97	0.46
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.51	0.45
1:C:84:HIS:CD2	1:C:137:THR:HG23	2.52	0.45
1:A:223:ASP:H	1:A:226:VAL:HG12	1.80	0.45
1:A:293:VAL:CG1	1:A:294:PRO:HD2	2.46	0.45
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.98	0.45
1:A:293:VAL:HG13	1:A:294:PRO:HD2	1.98	0.44
1:C:12:GLU:HG2	1:C:17:VAL:HG22	1.99	0.44
1:A:177:CYS:SG	1:A:179:TYR:O	2.67	0.44
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.82	0.44
3:C:1297:4SP:N1	3:C:1297:4SP:H22	2.32	0.44
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.99	0.43
1:A:156:VAL:HG11	1:A:181:SER:HB3	2.00	0.43
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.89	0.43
1:C:38:ASP:HB3	1:C:41:THR:OG1	2.18	0.43
1:C:98:GLY:HA2	1:C:199:ARG:HD3	2.00	0.43
1:C:119:HIS:HD2	6:D:2001:HOH:O	2.02	0.43
2:B:334[A]:MET:HE2	6:B:2078:HOH:O	2.19	0.42
2:B:177:ASP:CG	2:B:178:TYR:H	2.27	0.42
1:C:251:VAL:HG12	1:C:252:VAL:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:427:PRO:HB2	2:D:429:THR:O	2.19	0.42
2:B:177:ASP:HA	2:B:179:HIS:H	1.84	0.42
2:B:219:VAL:HG22	2:B:232:LEU:HD11	2.01	0.42
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.34	0.42
1:C:220:GLY:O	1:C:269:TYR:CZ	2.73	0.42
1:A:115:LEU:HD21	1:A:185:ASP:HB3	2.01	0.42
2:B:206:ILE:HG22	2:B:210:MET:HE1	2.02	0.41
2:D:227:LEU:HD12	2:D:261:MET:HE3	2.03	0.41
1:A:249:SER:HA	1:A:260:ARG:HD3	2.02	0.41
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.03	0.41
2:B:233:HIS:HD2	6:B:2068:HOH:O	2.03	0.41
2:B:282:THR:C	2:B:285:THR:N	2.78	0.40
1:C:137:THR:HG22	1:C:296:LEU:HD12	2.02	0.40
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.37	0.40
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.86	0.40
1:A:51:GLU:O	1:A:55:LEU:HB2	2.22	0.40
1:A:72:THR:HG22	1:A:73:GLU:H	1.87	0.40

There are no symmetry-related clashes.

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	294/302 (97%)	289 (98%)	4 (1%)	1 (0%)	36	35
1	C	267/302 (88%)	259 (97%)	7 (3%)	1 (0%)	30	27
2	B	255/260 (98%)	251 (98%)	3 (1%)	1 (0%)	30	27
2	D	254/260 (98%)	252 (99%)	2 (1%)	0	100	100
All	All	1070/1124 (95%)	1051 (98%)	16 (2%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	A	164	VAL
2	B	177	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/264 (100%)	249 (95%)	14 (5%)	20	18
1	C	238/264 (90%)	229 (96%)	9 (4%)	29	29
2	B	233/234 (100%)	220 (94%)	13 (6%)	19	16
2	D	230/234 (98%)	225 (98%)	5 (2%)	45	50
All	All	964/996 (97%)	923 (96%)	41 (4%)	28	25

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	34	LYS
1	A	55	LEU
1	A	56	LYS
1	A	71[A]	HIS
1	A	71[B]	HIS
1	A	74	ASN
1	A	101	LEU
1	A	148	LEU
1	A	150	ARG
1	A	206	ASP
1	A	230	VAL
1	A	248	PHE
1	A	255	LEU
2	B	177	ASP
2	B	232	LEU
2	B	285	THR
2	B	292	LEU
2	B	316	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	334[A]	MET
2	B	334[B]	MET
2	B	348	LEU
2	B	384	LEU
2	B	391	LEU
2	B	411[A]	GLU
2	B	411[B]	GLU
2	B	428	GLU
1	C	9	LYS
1	C	55	LEU
1	C	72[A]	THR
1	C	72[B]	THR
1	C	101	LEU
1	C	148	LEU
1	C	150	ARG
1	C	163	VAL
1	C	221	THR
2	D	232	LEU
2	D	292	LEU
2	D	348	LEU
2	D	391	LEU
2	D	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	119	HIS
1	A	265	GLN
2	B	228	GLN
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	425	ASN
1	C	60	HIS
1	C	62	ASN
1	C	84	HIS
1	C	119	HIS
1	C	265	GLN
2	D	179	HIS
2	D	183	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	254	GLN
2	D	313	GLN
2	D	317	GLN
2	D	395	HIS
2	D	403	GLN
2	D	415	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	0.87	0	10,14,16	1.04	0
1	TPO	C	160	1	8,10,11	0.92	0	10,14,16	0.94	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
1	TPO	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	4SP	C	1297	-	31,31,31	2.15	7 (22%)	43,44,44	2.34	14 (32%)
4	SGM	B	1433	-	5,5,5	0.66	0	5,5,5	0.89	0
3	4SP	A	1298	-	31,31,31	2.22	6 (19%)	43,44,44	1.84	9 (20%)
4	SGM	D	1433	-	5,5,5	0.42	0	5,5,5	0.44	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	4SP	C	1297	-	-	8/15/23/23	0/4/4/4
4	SGM	B	1433	-	-	3/4/4/4	-
3	4SP	A	1298	-	-	4/15/23/23	0/4/4/4
4	SGM	D	1433	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	4SP	C20-S23	-9.21	1.62	1.77
3	C	1297	4SP	C20-S23	-8.57	1.63	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	4SP	S23-N26	-4.12	1.52	1.60
3	C	1297	4SP	S23-N26	-3.86	1.53	1.60
3	C	1297	4SP	C5-C6	3.27	1.47	1.41
3	A	1298	4SP	C5-C6	3.24	1.47	1.41
3	C	1297	4SP	O25-S23	2.81	1.48	1.43
3	A	1298	4SP	C6-N1	2.63	1.36	1.32
3	C	1297	4SP	C5-N7	-2.58	1.34	1.39
3	A	1298	4SP	O24-S23	2.46	1.48	1.43
3	C	1297	4SP	C6-N1	2.33	1.35	1.32
3	C	1297	4SP	O24-S23	2.30	1.47	1.43
3	A	1298	4SP	C5-N7	-2.18	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297	4SP	O25-S23-O24	-7.68	106.98	118.80
3	A	1298	4SP	O25-S23-O24	-5.41	110.47	118.80
3	C	1297	4SP	C2-N1-C6	4.28	122.75	115.38
3	C	1297	4SP	C5-C4-N3	-4.25	122.38	126.55
3	C	1297	4SP	C5-C6-N1	-4.04	118.08	123.49
3	A	1298	4SP	C5-C4-N3	-3.94	122.69	126.55
3	C	1297	4SP	N3-C2-N1	-3.82	119.99	126.26
3	C	1297	4SP	O25-S23-C20	3.81	111.66	107.35
3	A	1298	4SP	C5-C6-N1	-3.59	118.68	123.49
3	A	1298	4SP	C2-N1-C6	3.59	121.56	115.38
3	C	1297	4SP	C5-N7-C8	3.27	107.17	103.48
3	A	1298	4SP	N3-C2-N1	-3.16	121.07	126.26
3	A	1298	4SP	O6-C6-C5	3.03	120.73	116.73
3	C	1297	4SP	N9-C8-N7	-2.78	109.63	113.87
3	A	1298	4SP	C15-C16-C11	-2.78	106.24	112.08
3	C	1297	4SP	C16-C11-C12	2.71	115.92	109.29
3	C	1297	4SP	O24-S23-N26	2.55	111.03	107.35
3	C	1297	4SP	C15-C16-C11	2.45	117.24	112.08
3	A	1298	4SP	C5-C4-N9	2.45	108.94	105.67
3	C	1297	4SP	O6-C6-N1	2.19	122.94	120.02
3	C	1297	4SP	C21-C20-C19	-2.11	117.72	120.47
3	A	1298	4SP	C5-N7-C8	2.05	105.80	103.48
3	C	1297	4SP	C5-C4-N9	2.03	108.39	105.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

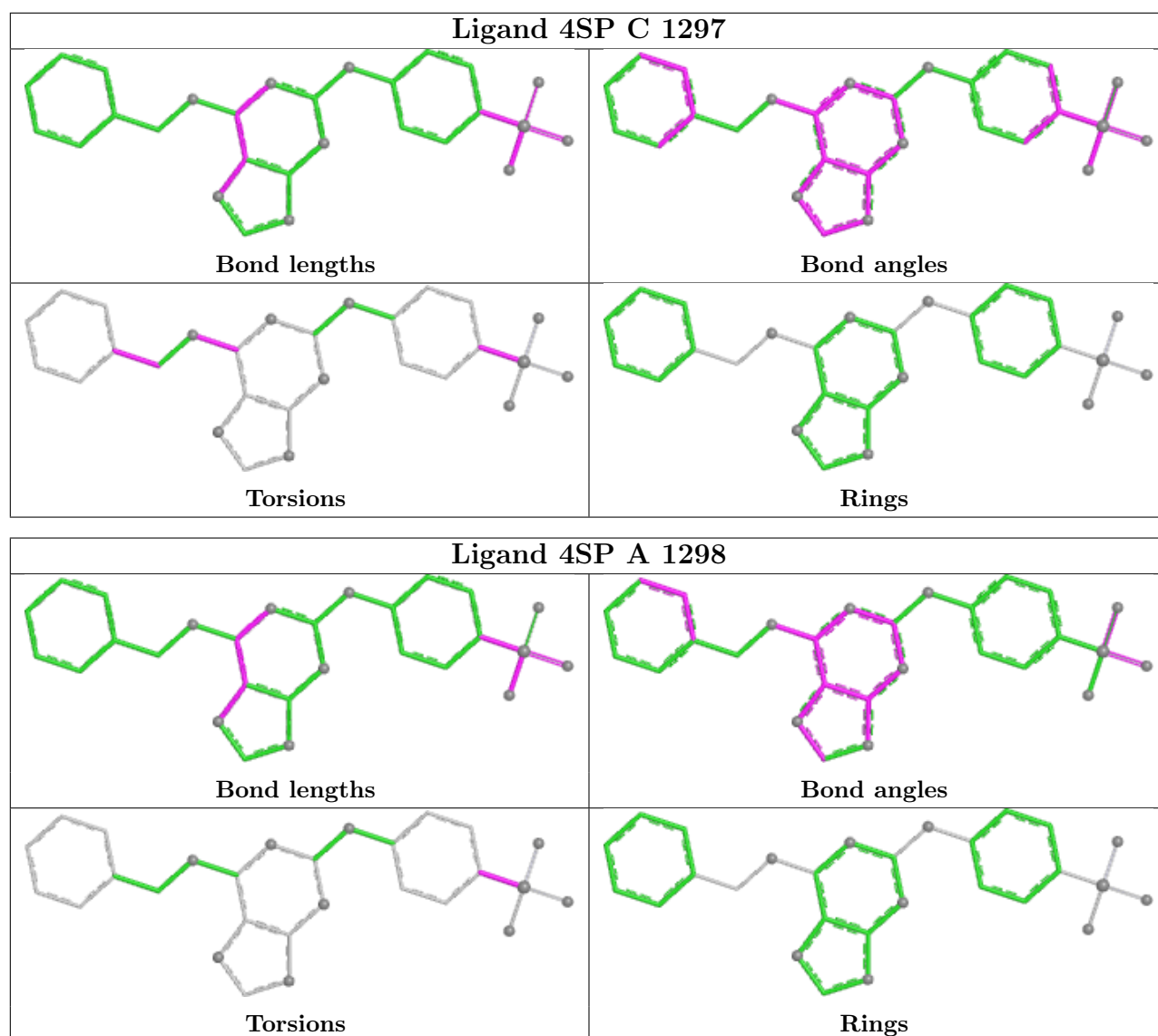
Mol	Chain	Res	Type	Atoms
4	B	1433	SGM	O2-C2-C3-O3
3	A	1298	4SP	C19-C20-S23-N26
3	C	1297	4SP	C19-C20-S23-O24
3	C	1297	4SP	C21-C20-S23-O24
4	B	1433	SGM	C1-C2-C3-O3
3	A	1298	4SP	C21-C20-S23-O24
3	C	1297	4SP	O6-C10-C11-C12
3	C	1297	4SP	O6-C10-C11-C16
3	A	1298	4SP	C21-C20-S23-N26
3	C	1297	4SP	C5-C6-O6-C10
4	B	1433	SGM	S1-C1-C2-O2
3	A	1298	4SP	C19-C20-S23-O24
3	C	1297	4SP	C21-C20-S23-N26
3	C	1297	4SP	C19-C20-S23-N26
3	C	1297	4SP	N1-C6-O6-C10

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	4SP	1	0
3	A	1298	4SP	2	0
4	D	1433	SGM	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 ⓘ

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	293/302 (97%)	1.03	39 (13%) 7 6	17, 35, 45, 51	5 (1%)
1	C	268/302 (88%)	1.48	65 (24%) 2 1	15, 35, 43, 47	3 (1%)
2	B	255/260 (98%)	0.88	22 (8%) 16 15	16, 35, 43, 51	4 (1%)
2	D	255/260 (98%)	1.78	83 (32%) 1 1	15, 36, 43, 50	1 (0%)
All	All	1071/1124 (95%)	1.29	209 (19%) 3 3	15, 35, 44, 51	13 (1%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72[A]	THR	10.2
2	B	431	ASN	6.6
1	C	256	ASP	6.4
1	A	59[A]	ASN	6.3
2	D	432	LEU	6.1
2	D	429	THR	6.1
1	C	186[A]	ILE	5.7
1	C	295	HIS	5.6
2	B	334[A]	MET	5.5
2	B	209[A]	SER	5.4
1	C	71[A]	HIS	5.4
1	A	71[A]	HIS	5.3
1	A	272[A]	ASN	5.3
1	C	251	VAL	5.2
1	C	253	PRO	4.9
2	D	367	VAL	4.9
1	C	222	PRO	4.9
2	D	250[A]	ARG	4.9
1	A	268[A]	HIS	4.8
1	A	97	THR	4.8
2	D	401	ALA	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	281	ILE	4.4
1	C	163	VAL	4.3
1	A	95	ALA	4.3
2	D	324	PRO	4.2
1	A	96	LEU	4.1
1	C	220	GLY	4.1
2	D	373	PRO	4.1
2	B	285	THR	3.9
2	B	411[A]	GLU	3.9
1	A	74	ASN	3.9
1	C	287	GLN	3.9
1	A	247	ASP	3.8
1	C	221	THR	3.8
1	A	179	TYR	3.8
1	C	74	ASN	3.8
2	B	374[A]	GLU	3.8
2	D	334	MET	3.8
2	D	288	LYS	3.7
1	A	8[A]	GLU	3.7
2	D	384	LEU	3.7
1	C	97	THR	3.7
2	D	251	GLY	3.6
1	C	282	ALA	3.6
1	C	296	LEU	3.6
2	D	431	ASN	3.6
2	D	372	TRP	3.5
1	C	44	VAL	3.5
2	D	363	ALA	3.5
1	C	37	LEU	3.5
2	B	178	TYR	3.5
2	D	286	TYR	3.5
2	D	405	ALA	3.5
1	C	39	THR	3.5
2	D	285	THR	3.5
2	B	323	GLN	3.5
1	C	102	PRO	3.5
2	B	176	PRO	3.4
2	D	371	SER	3.4
2	D	287	THR	3.4
1	A	178	LYS	3.3
2	D	179	HIS	3.3
2	D	264	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	276	ALA	3.3
1	A	2	GLU	3.3
2	D	225	TYR	3.3
2	D	280	TYR	3.3
2	D	278	PHE	3.3
2	D	282	THR	3.2
2	D	327	CYS	3.2
2	D	320	LEU	3.2
1	A	72	THR	3.2
1	C	2	GLU	3.1
2	B	179	HIS	3.1
2	D	319	PHE	3.1
1	C	41	THR	3.1
1	C	162	GLU	3.1
1	C	217	ARG	3.1
2	D	325	ALA	3.1
2	B	429	THR	3.0
2	B	177	ASP	3.0
1	A	230	VAL	3.0
1	C	156	VAL	3.0
1	C	175	LEU	3.0
1	C	70	ILE	3.0
1	C	43	GLY	3.0
1	C	76	LEU	3.0
2	D	262	LEU	3.0
2	D	430	LEU	3.0
1	C	161	HIS	3.0
1	C	3	ASN	2.9
2	D	376	LEU	2.9
1	A	163	VAL	2.9
2	D	402	PRO	2.9
1	A	226	VAL	2.9
2	D	181	ASP	2.9
2	D	326	ASN	2.9
1	A	73	GLU	2.8
2	D	410	ARG	2.8
2	D	271	TYR	2.8
2	D	270	ILE	2.8
1	C	25	LEU	2.7
2	D	292	LEU	2.7
2	D	323	GLN	2.7
2	B	428	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	398	TYR	2.7
1	A	162	GLU	2.7
1	C	79	VAL	2.7
1	C	84	HIS	2.7
2	D	420	GLY	2.7
1	C	165	THR	2.7
2	D	294	MET	2.7
1	C	49	ILE	2.7
2	B	369	GLY	2.6
1	C	131	GLN	2.6
2	B	324	PRO	2.6
1	A	181	SER	2.6
2	D	332	LEU	2.6
1	A	246	GLN	2.5
2	D	395	HIS	2.5
1	A	6	LYS	2.5
1	A	36	ARG	2.5
2	D	273	PRO	2.5
2	B	432	LEU	2.5
1	C	52	ILE	2.5
1	C	293	VAL	2.5
2	D	298	VAL	2.5
1	A	0	SER	2.5
2	D	375	SER	2.5
2	D	427	PRO	2.5
1	A	296	LEU	2.5
1	A	248	PHE	2.5
1	C	88	LYS	2.5
1	A	297	ARG	2.5
2	D	360	PHE	2.5
1	C	289	VAL	2.4
2	B	281	ILE	2.5
2	D	301	VAL	2.4
1	C	258	ASP	2.4
1	A	177	CYS	2.4
2	D	193	CYS	2.4
1	C	151	ALA	2.4
1	C	255	LEU	2.4
2	D	218	LEU	2.4
1	A	256	ASP	2.4
1	C	254	PRO	2.4
1	C	294	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	418	TYR	2.4
2	D	423	LEU	2.4
1	C	46	SER	2.4
1	C	77	TYR	2.3
1	C	157	ARG	2.3
1	C	252	VAL	2.3
1	C	290	THR	2.3
1	C	138	GLU	2.3
2	B	274	GLU	2.3
1	A	5	GLN	2.3
2	B	198	GLY	2.3
1	C	288	ASP	2.3
2	D	293	ARG	2.3
2	D	192	LYS	2.3
1	A	161	HIS	2.3
2	D	197	VAL	2.3
1	A	183	ALA	2.3
1	C	75	LYS	2.3
2	D	198	GLY	2.3
2	D	369	GLY	2.3
1	C	96	LEU	2.3
1	A	19	TYR	2.3
2	D	322	GLN	2.2
1	C	35	ILE	2.2
2	D	377	ILE	2.2
2	D	256	VAL	2.2
2	D	284	ASP	2.2
2	D	425	ASN	2.2
2	D	221	VAL	2.2
2	D	260	ALA	2.2
1	C	219	LEU	2.2
2	D	255	LEU	2.2
2	B	280	TYR	2.2
1	C	56	LYS	2.2
1	A	7	VAL	2.2
1	C	73	GLU	2.2
2	D	180	GLU	2.2
1	C	95	ALA	2.2
1	A	242	LYS	2.2
2	D	283	ASP	2.2
2	D	346	PRO	2.1
1	C	209	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	409	ILE	2.1
2	D	291	VAL	2.1
1	A	229	GLY	2.1
2	D	254	GLN	2.1
1	A	237	LYS	2.1
1	C	199	ARG	2.1
2	B	182	ILE	2.1
1	C	0	SER	2.1
2	D	249	LEU	2.1
1	A	293	VAL	2.1
1	A	42	GLU	2.0
2	D	245	SER	2.1
2	D	277	GLU	2.0
2	D	403	GLN	2.0
2	B	282	THR	2.0
2	D	258	THR	2.0
1	C	159	TYR	2.0
2	D	201	LYS	2.0
1	C	17	VAL	2.0
2	D	392	MET	2.0

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	0.91	0.12	28,32,35,35	0
1	TPO	A	160	11/12	0.96	0.10	29,33,35,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

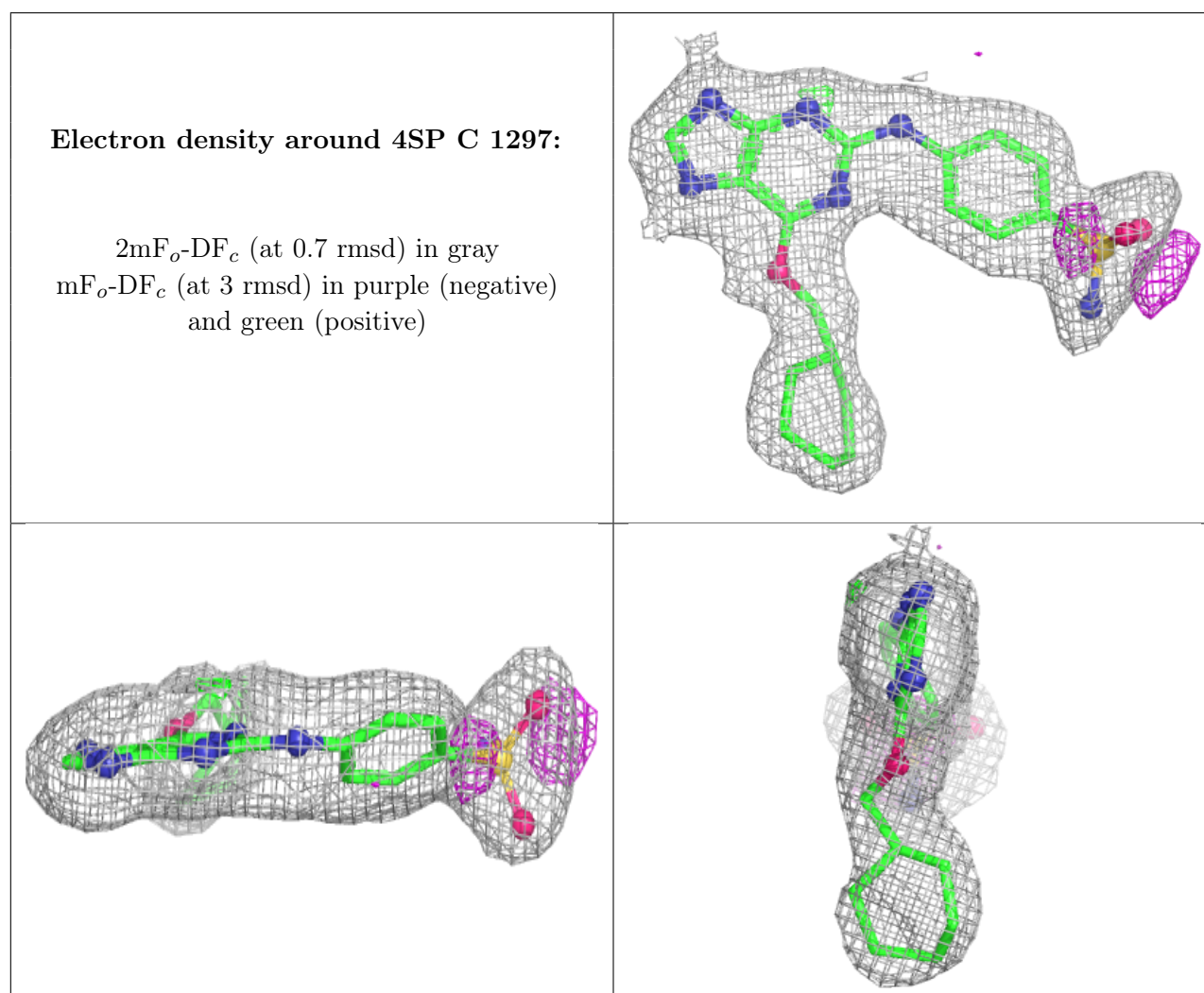
6.4 Ligands [i](#)

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.

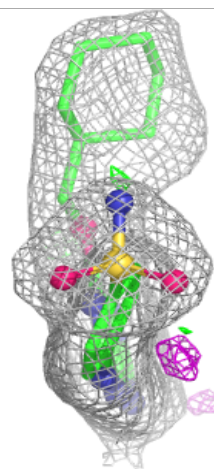
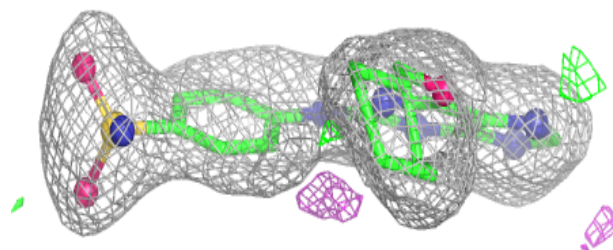
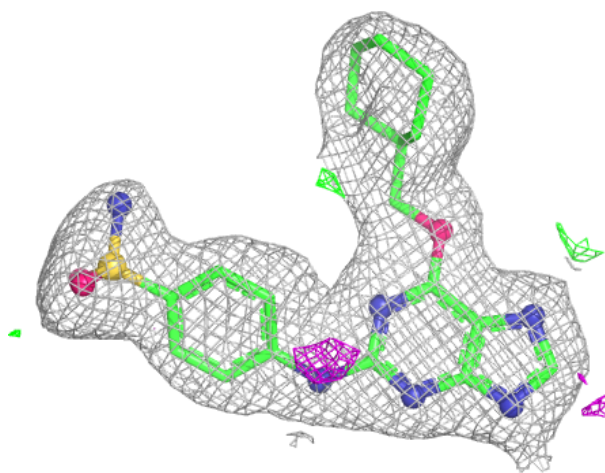
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SGM	D	1433	6/6	0.78	0.23	66,67,68,69	0
4	SGM	B	1433	6/6	0.91	0.18	45,52,54,55	0
3	4SP	C	1297	28/28	0.92	0.09	33,35,39,40	0
5	MG	B	1434	1/1	0.94	0.20	43,43,43,43	0
3	4SP	A	1298	28/28	0.95	0.09	35,38,45,45	0
5	MG	D	1434	1/1	0.95	0.18	38,38,38,38	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 4SP A 1298:

$2mF_o-DF_c$ (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.