



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:31 am BST

PDB ID : 2IW9
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

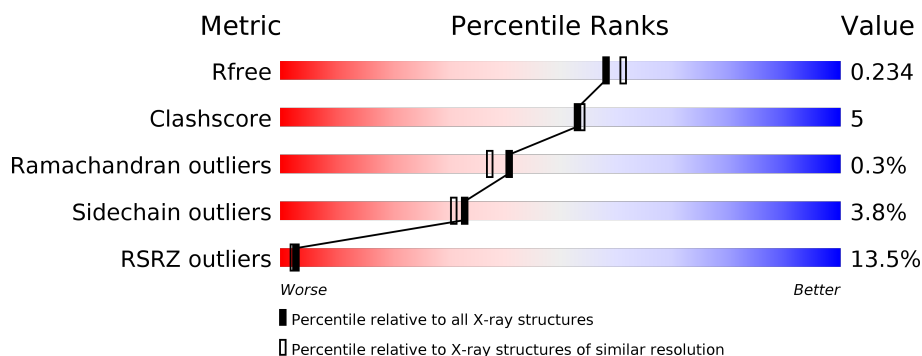
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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

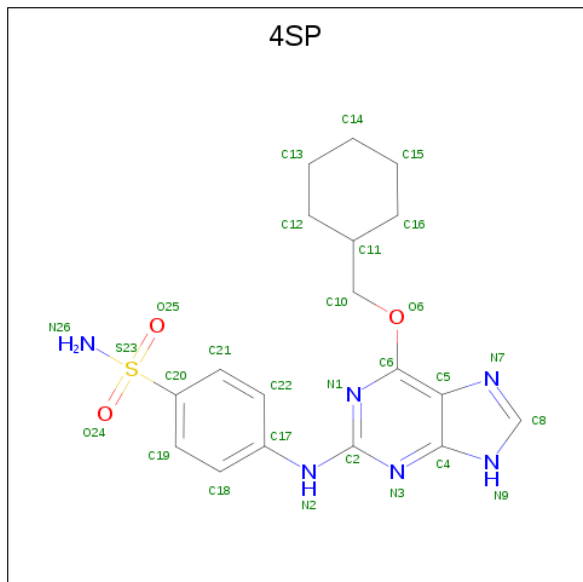
- Molecule 2 is a protein called CYCLIN-A2.

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:

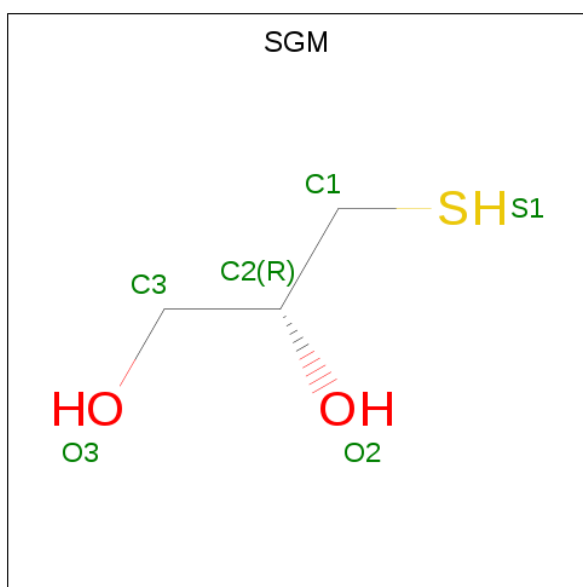
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	expression tag	UNP P20248
D	173	MET	-	expression tag	UNP P20248

- Molecule 3 is O6-CYCLOHEXYLMETHOXY-2-(4'-SULPHAMOYLANILINO) PURINE (three-letter code: 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 (three-letter code: 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 (three-letter code: 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		

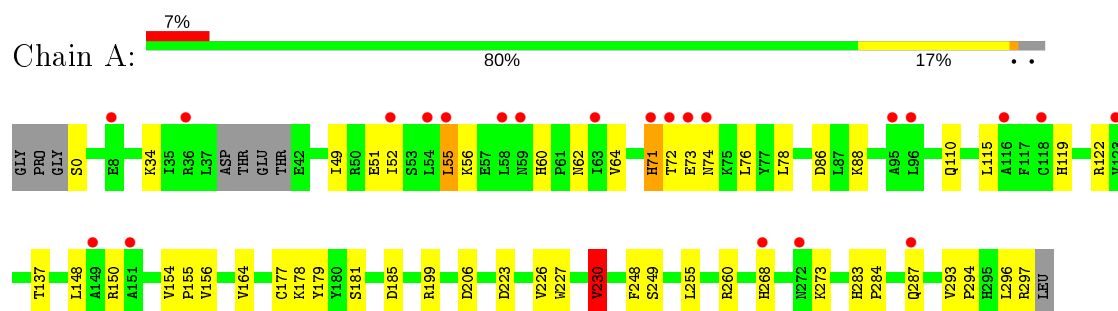
- Molecule 6 is water.

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		

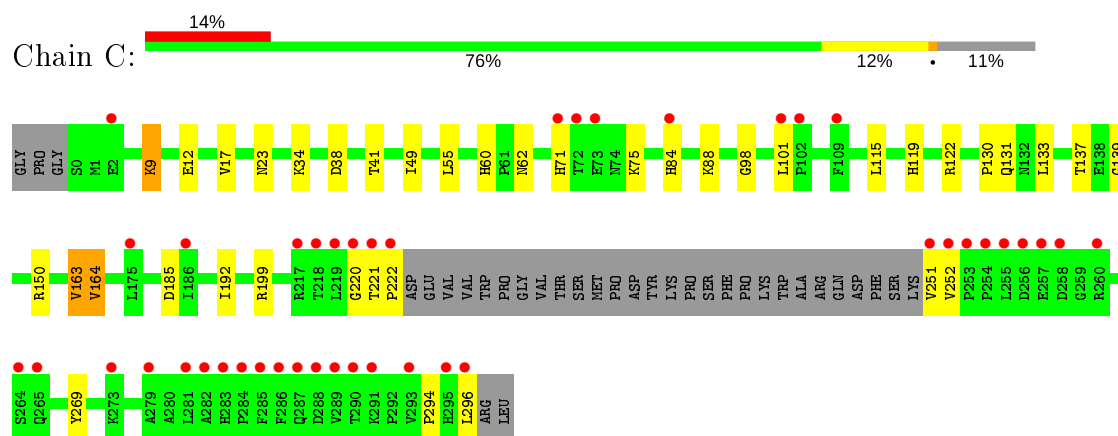
3 Residue-property plots [i](#)

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

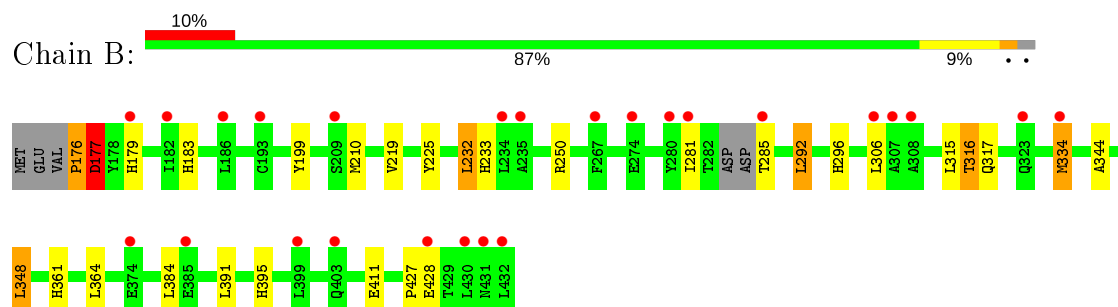
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



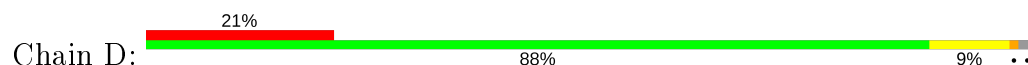
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

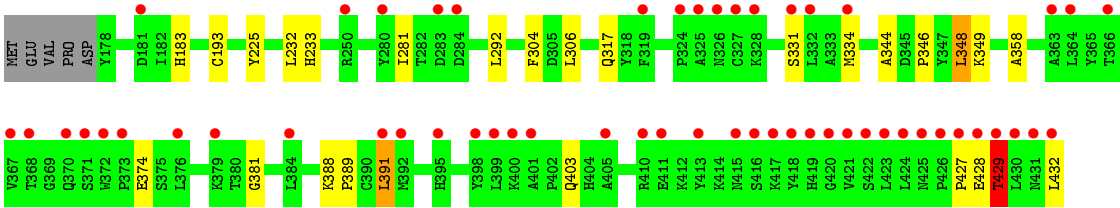


• Molecule 2: CYCLIN-A2



• 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 47.04 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (100.00-2.00) 97.6 (47.04-2.00)	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 , 54.7	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	0.94	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: TPO, MG, SGM, 4SP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	0/2462	0.70	2/3339 (0.1%)
1	C	0.44	0/2217	0.58	0/3006
2	B	0.54	0/2141	0.60	1/2903 (0.0%)
2	D	0.86	7/2121 (0.3%)	0.61	1/2878 (0.0%)
All	All	0.62	7/8941 (0.1%)	0.63	4/12126 (0.0%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	374	GLU	CD-OE1	18.38	1.45	1.25
2	D	374	GLU	CD-OE2	18.13	1.45	1.25
2	D	429	THR	C-O	13.29	1.48	1.23
2	D	429	THR	C-N	8.42	1.53	1.34
2	D	403	GLN	CD-OE1	6.74	1.38	1.24
2	D	381	GLY	C-O	5.93	1.33	1.23
2	D	428	GLU	C-O	5.26	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	374	GLU	OE1-CD-OE2	9.90	135.18	123.30
1	A	230	VAL	CB-CA-C	-6.00	100.01	111.40
1	A	199	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	B	364	LEU	CA-CB-CG	5.09	127.01	115.30

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 [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	2391	0	2424	38	0
1	C	2166	0	2217	25	0
2	B	2076	0	2099	27	0
2	D	2068	0	2096	12	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	95	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 5.

All (95) 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
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: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:210:MET:HE1	2:B:250:ARG:HB2	1.79	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
1:C:220:GLY:O	1:C:269:TYR:OH	2.08	0.58
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:B:210:MET:HE1	2:B:250:ARG:CB	2.35	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:N	2.60	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
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
1:A:119:HIS:HD2	6:B:2013:HOH:O	1.93	0.51
2:B:315:LEU:HD12	2:B:334[A]:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:177:ASP:C	2:B:179:HIS:H	2.15	0.49
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
1:C:133:LEU:HD11	1:C:192:ILE:HD13	1.94	0.48
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.95	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
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
2:B:334[A]:MET:HE2	6:B:2078:HOH:O	2.15	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:D:331:SER:HA	2:D:334:MET:HE2	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:ASP:H22	3:C:1297:ASP:N1	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:HA	2:B:292:LEU:HD12	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
1:C:251:VAL:HG12	1:C:252:VAL:HG23	2.02	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:SER:HA	1:A:260:ARG:HD3	2.02	0.41
2:B:315:LEU:CD1	2:B:334[A]:MET:HE3	2.50	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
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
2:B:315:LEU:HD12	2:B:334[A]:MET:CE	2.51	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 [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	294/302 (97%)	289 (98%)	4 (1%)	1 (0%)	41	37
1	C	267/302 (88%)	259 (97%)	7 (3%)	1 (0%)	34	30
2	B	255/260 (98%)	251 (98%)	3 (1%)	1 (0%)	34	30
2	D	254/260 (98%)	252 (99%)	2 (1%)	0	100	100
All	All	1070/1124 (95%)	1051 (98%)	16 (2%)	3 (0%)	41	37

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 ⓘ

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%)	22	18
1	C	238/264 (90%)	231 (97%)	7 (3%)	42	43
2	B	233/234 (100%)	220 (94%)	13 (6%)	21	17
2	D	230/234 (98%)	225 (98%)	5 (2%)	52	55
All	All	964/996 (97%)	925 (96%)	39 (4%)	33	29

All (39) 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	122	ARG
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	199	TYR
2	B	232	LEU
2	B	285	THR
2	B	292	LEU
2	B	316	THR
2	B	334[A]	MET
2	B	334[B]	MET
2	B	348	LEU
2	B	384	LEU

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Mol	Chain	Res	Type
2	B	411[A]	GLU
2	B	411[B]	GLU
2	B	428	GLU
1	C	9	LYS
1	C	55	LEU
1	C	101	LEU
1	C	122	ARG
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

Some 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	85	GLN
1	A	119	HIS
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
1	C	60	HIS
1	C	62	ASN
1	C	84	HIS
1	C	119	HIS
1	C	265	GLN
1	C	268	HIS
2	D	179	HIS
2	D	183	HIS
2	D	254	GLN
2	D	317	GLN
2	D	395	HIS
2	D	403	GLN

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	0.86	0	10,14,16	1.01	0
1	TPO	C	160	1	8,10,11	0.90	0	10,14,16	0.93	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
4	SGM	D	1433	-	5,5,5	0.41	0	5,5,5	0.42	0
3	4SP	C	1297	-	28,31,31	2.08	6 (21%)	35,44,44	2.43	13 (37%)
4	SGM	B	1433	-	5,5,5	0.65	0	5,5,5	0.86	0
3	4SP	A	1298	-	28,31,31	2.15	4 (14%)	35,44,44	1.78	7 (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
4	SGM	D	1433	-	-	0/4/4/4	-
3	4SP	C	1297	-	-	9/15/23/23	0/4/4/4
4	SGM	B	1433	-	-	3/4/4/4	-
3	4SP	A	1298	-	-	4/15/23/23	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	4SP	C20-S23	-9.03	1.62	1.77
3	C	1297	4SP	C20-S23	-8.40	1.63	1.77
3	A	1298	4SP	S23-N26	-4.04	1.52	1.60
3	C	1297	4SP	S23-N26	-3.78	1.53	1.60
3	C	1297	4SP	O25-S23	2.66	1.48	1.43
3	A	1298	4SP	C6-N1	2.60	1.36	1.31
3	C	1297	4SP	C6-N1	2.35	1.35	1.31
3	A	1298	4SP	O24-S23	2.33	1.48	1.43
3	C	1297	4SP	O6-C6	2.28	1.37	1.35
3	C	1297	4SP	O24-S23	2.17	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297	4SP	O25-S23-O24	-7.16	106.98	118.76
3	A	1298	4SP	O25-S23-O24	-5.04	110.47	118.76
3	C	1297	4SP	C2-N1-C6	4.29	122.75	115.18
3	C	1297	4SP	C2-N3-C4	4.21	120.06	115.28
3	C	1297	4SP	N3-C2-N1	-3.94	119.99	126.23
3	A	1298	4SP	C2-N3-C4	3.91	119.72	115.28
3	C	1297	4SP	O25-S23-C20	3.86	111.66	107.35
3	C	1297	4SP	C10-O6-C6	3.68	121.02	117.50
3	A	1298	4SP	C2-N1-C6	3.61	121.56	115.18
3	C	1297	4SP	O6-C6-N1	3.26	122.94	120.12
3	A	1298	4SP	N3-C2-N1	-3.26	121.07	126.23
3	A	1298	4SP	C15-C16-C11	-3.13	106.24	112.15
3	C	1297	4SP	C5-C6-N1	-2.72	118.08	123.26
3	C	1297	4SP	C16-C11-C12	2.70	115.92	109.33
3	C	1297	4SP	C15-C16-C11	2.69	117.24	112.15
3	C	1297	4SP	O24-S23-N26	2.47	111.03	107.36
3	A	1298	4SP	C5-C6-N1	-2.40	118.68	123.26
3	C	1297	4SP	O6-C10-C11	2.23	114.02	108.21
3	C	1297	4SP	C13-C12-C11	2.15	116.22	112.15
3	A	1298	4SP	C10-O6-C6	-2.10	115.50	117.50

There are no chirality outliers.

All (16) torsion outliers are listed below:

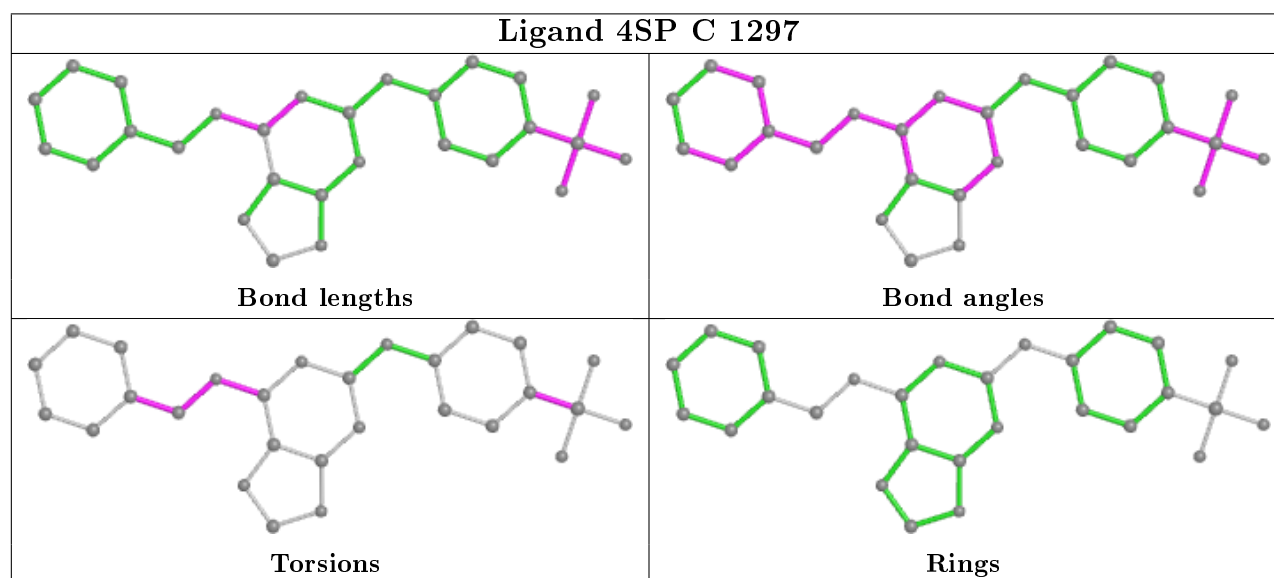
Mol	Chain	Res	Type	Atoms
4	B	1433	SGM	O2-C2-C3-O3
3	C	1297	4SP	C21-C20-S23-O24
3	C	1297	4SP	C11-C10-O6-C6
3	C	1297	4SP	C19-C20-S23-O24
3	A	1298	4SP	C19-C20-S23-N26
3	A	1298	4SP	C21-C20-S23-N26
3	A	1298	4SP	C21-C20-S23-O24
4	B	1433	SGM	C1-C2-C3-O3
4	B	1433	SGM	S1-C1-C2-O2
3	C	1297	4SP	O6-C10-C11-C12
3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

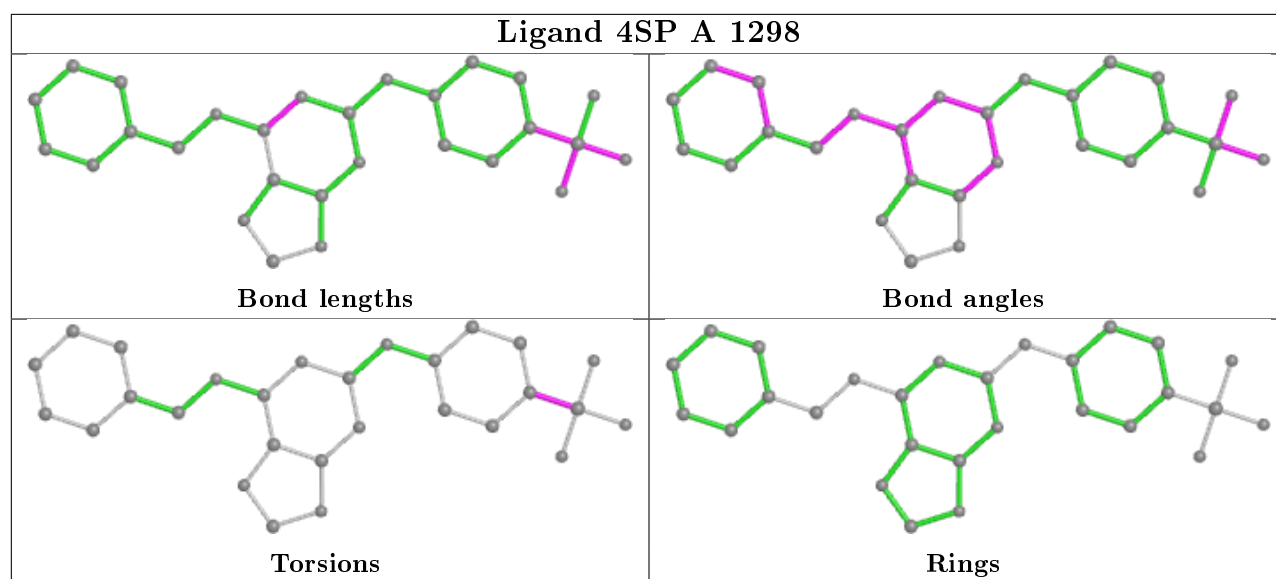
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1433	SGM	1	0
3	C	1297	4SP	1	0
3	A	1298	4SP	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(Å ²)	Q<0.9
1	A	293/302 (97%)	0.76	22 (7%) 14 13	29, 35, 45, 51	5 (1%)
1	C	268/302 (88%)	1.02	43 (16%) 1 1	27, 35, 43, 47	3 (1%)
2	B	255/260 (98%)	0.79	25 (9%) 7 7	30, 35, 43, 51	4 (1%)
2	D	255/260 (98%)	1.21	55 (21%) 0 0	30, 36, 43, 50	1 (0%)
All	All	1071/1124 (95%)	0.94	145 (13%) 3 2	27, 35, 44, 51	13 (1%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	14.4
2	D	367	VAL	10.8
2	D	423	LEU	8.4
1	C	287	GLN	7.9
2	D	324	PRO	6.9
1	C	221	THR	6.7
1	C	222	PRO	6.5
1	C	251	VAL	6.2
1	A	59[A]	ASN	6.1
1	C	253	PRO	6.0
1	C	256	ASP	5.9
2	B	431	ASN	5.6
2	D	430	LEU	5.2
1	C	282	ALA	5.2
1	C	296	LEU	5.2
2	D	368	THR	5.0
2	B	323	GLN	5.0
2	D	415	ASN	4.9
1	A	71[A]	HIS	4.8
2	D	327	CYS	4.7
2	D	326	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	186[A]	ILE	4.4
2	D	401	ALA	4.4
1	C	258	ASP	4.4
1	C	288	ASP	4.3
2	D	421	VAL	4.3
2	B	432	LEU	4.3
2	D	427	PRO	4.3
1	C	295	HIS	4.3
2	D	428	GLU	4.2
2	D	429	THR	4.2
1	C	289	VAL	4.1
2	D	284	ASP	4.1
2	D	371	SER	4.0
2	D	332	LEU	4.0
2	D	325	ALA	3.9
2	D	416	SER	3.9
2	B	234	LEU	3.9
1	C	284	PRO	3.9
1	A	96	LEU	3.8
2	D	431	ASN	3.8
1	C	102	PRO	3.8
2	D	398	TYR	3.8
1	C	293	VAL	3.7
1	C	286	PHE	3.7
1	C	290	THR	3.7
1	A	272[A]	ASN	3.7
2	D	372	TRP	3.7
1	A	73	GLU	3.6
2	B	334[A]	MET	3.6
2	D	384	LEU	3.6
1	C	257	GLU	3.5
1	C	291	LYS	3.5
1	A	74	ASN	3.4
2	B	209[A]	SER	3.4
2	B	280	TYR	3.4
1	C	260	ARG	3.4
2	D	399	LEU	3.4
2	D	420	GLY	3.4
1	C	285	PHE	3.4
2	D	422	SER	3.3
2	D	319	PHE	3.3
2	D	419	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	285	THR	3.3
2	D	410	ARG	3.3
1	C	73	GLU	3.3
2	D	363	ALA	3.3
1	C	273	LYS	3.2
2	B	267	PHE	3.2
1	C	2	GLU	3.1
1	C	283	HIS	3.1
2	D	395	HIS	3.1
1	A	95	ALA	3.1
2	D	328	LYS	3.0
2	D	283	ASP	3.0
2	D	413	TYR	3.0
2	D	400	LYS	3.0
1	C	255	LEU	2.9
1	C	72[A]	THR	2.9
2	D	424	LEU	2.9
2	D	334	MET	2.9
1	C	109	PHE	2.8
1	A	36	ARG	2.8
1	C	219	LEU	2.8
2	D	426	PRO	2.7
2	D	418	TYR	2.7
2	D	366	THR	2.7
2	D	391	LEU	2.7
1	C	217	ARG	2.7
1	C	175	LEU	2.7
2	D	331	SER	2.6
1	A	287	GLN	2.6
1	C	254	PRO	2.6
2	D	392	MET	2.6
1	C	252	VAL	2.6
1	A	54	LEU	2.6
2	B	235	ALA	2.6
1	A	151	ALA	2.5
1	C	279	ALA	2.5
1	A	118	CYS	2.5
2	B	428	GLU	2.5
1	A	123	VAL	2.5
2	D	280	TYR	2.5
1	A	55	LEU	2.5
2	D	250[A]	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	425	ASN	2.5
1	C	281	LEU	2.4
2	D	373	PRO	2.4
1	C	84	HIS	2.4
2	D	411	GLU	2.4
2	B	306	LEU	2.4
2	D	417	LYS	2.4
2	B	374[A]	GLU	2.4
2	B	430	LEU	2.3
1	A	149	ALA	2.3
2	D	364	LEU	2.3
1	C	220	GLY	2.3
1	A	72	THR	2.3
1	A	52	ILE	2.3
1	C	264	SER	2.3
1	A	116	ALA	2.3
2	B	403	GLN	2.3
1	C	265	GLN	2.3
2	B	281	ILE	2.2
2	B	385	GLU	2.2
1	C	218	THR	2.2
2	D	379	LYS	2.2
2	B	274	GLU	2.2
1	A	8[A]	GLU	2.2
1	C	71[A]	HIS	2.1
2	B	179	HIS	2.1
2	B	193	CYS	2.1
1	A	63	ILE	2.1
2	B	186	LEU	2.1
2	D	376	LEU	2.1
2	D	370	GLN	2.1
1	A	58	LEU	2.1
2	B	307	ALA	2.1
2	D	181	ASP	2.1
2	D	405	ALA	2.1
1	C	101	LEU	2.0
2	B	399	LEU	2.0
2	B	182	ILE	2.0
1	A	268[A]	HIS	2.0
2	B	308	ALA	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	0.94	0.12	28,32,35,35	0
1	TPO	A	160	11/12	0.98	0.13	29,33,35,36	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

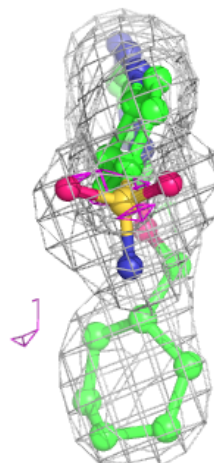
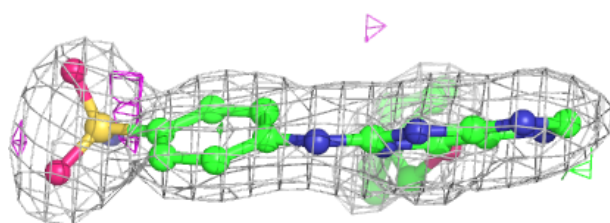
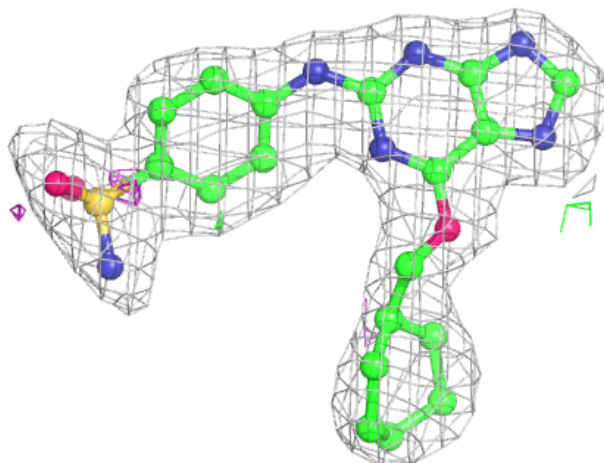
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

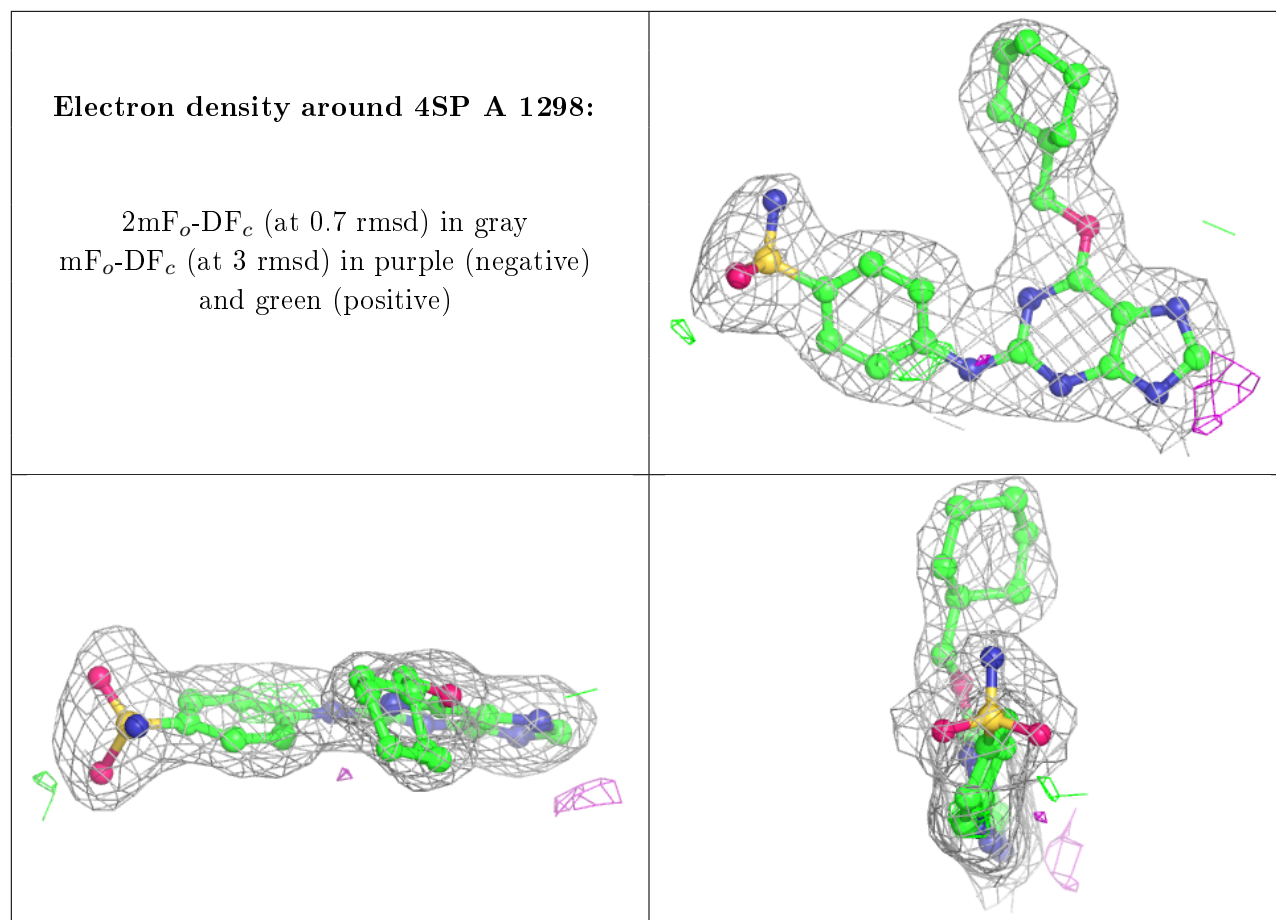
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SGM	D	1433	6/6	0.77	0.19	66,67,68,69	0
3	4SP	C	1297	28/28	0.92	0.14	33,35,39,40	0
5	MG	D	1434	1/1	0.92	0.15	38,38,38,38	0
5	MG	B	1434	1/1	0.92	0.19	43,43,43,43	0
4	SGM	B	1433	6/6	0.94	0.14	45,52,54,55	0
3	4SP	A	1298	28/28	0.96	0.14	35,38,45,45	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 C 1297:

$2mF_o-DF_c$ (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.