



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:26 PM UTC

PDB ID : 1OI9 / pdb_00001oi9
Title : Structure of human Thr160-phospho CDK2/cyclin A complexed with a 6-cyclohexylmethoxy-2-anilino-purine inhibitor
Authors : Pratt, D.J.; Endicott, J.A.; Noble, M.E.M.
Deposited on : 2003-06-10
Resolution : 2.10 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:

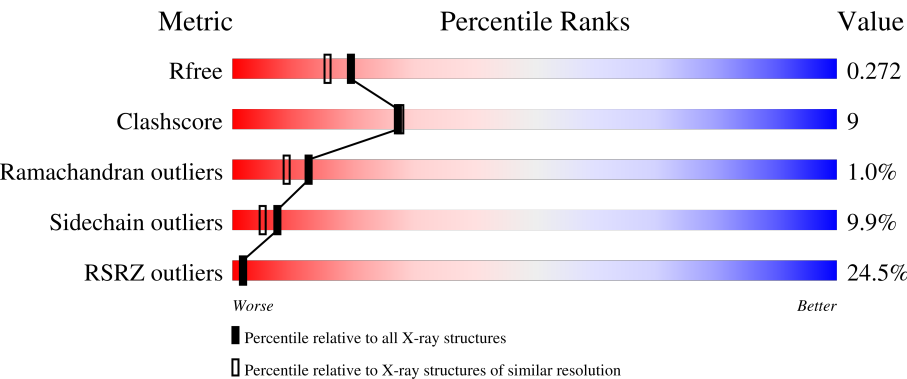
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	6% 74% 21% ..
1	C	302	44% 65% 28% 5% .
2	B	260	3% 83% 13% ..
2	D	260	43% 74% 20% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9318 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.

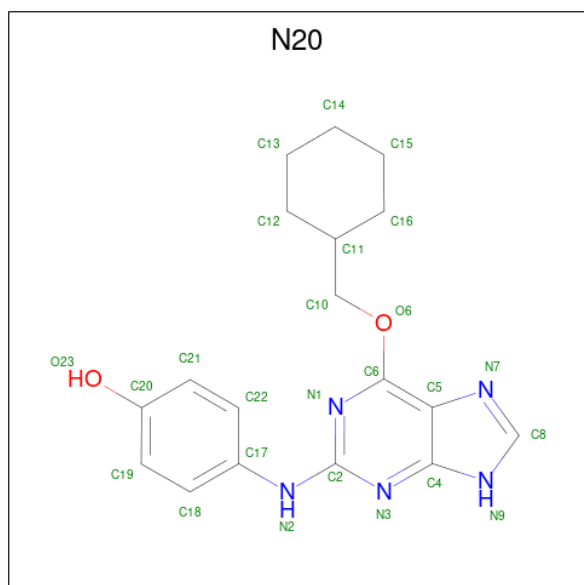
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	3	0
			2388	1549	404	426	1	8			
1	C	297	Total	C	N	O	P	S	0	1	0
			2392	1552	405	426	1	8			

- Molecule 2 is a protein called CYCLIN A2.

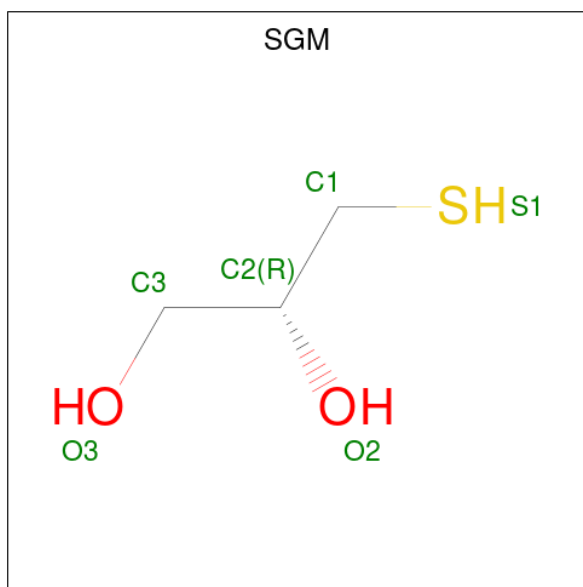
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	2	0
			2089	1354	339	383	13			
2	D	253	Total	C	N	O	S	0	0	0
			2045	1326	333	375	11			

- Molecule 3 is 6-CYCLOHEXYLMETHYLOXY-2-(4'-HYDROXYANILINO)PURINE (CCD ID: N20) (formula: $C_{18}H_{21}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	18	5	2		
3	C	1	Total	C	N	O	0	0
			25	18	5	2		

- 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		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	144	Total	O	0	0
			144	144		
6	B	132	Total	O	0	0
			132	132		

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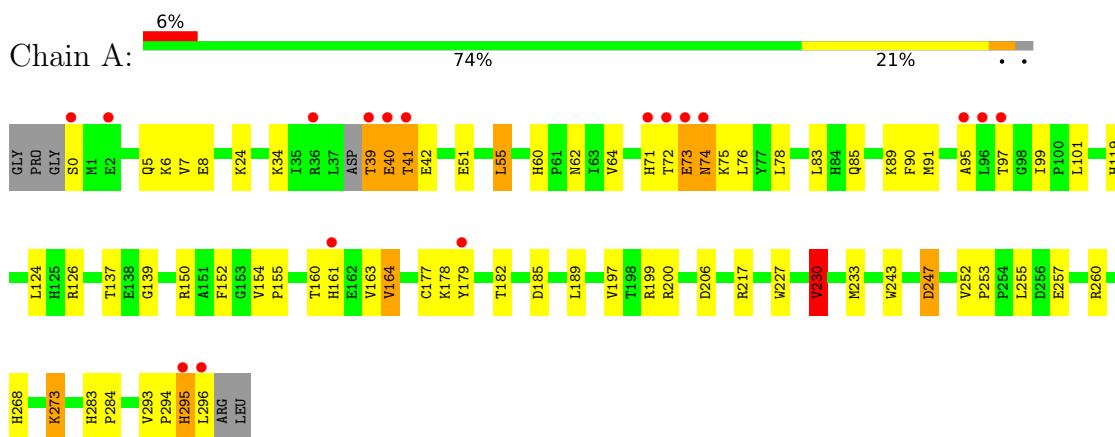
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	41	Total	O	0	0
			41	41		
6	D	24	Total	O	0	0
			24	24		

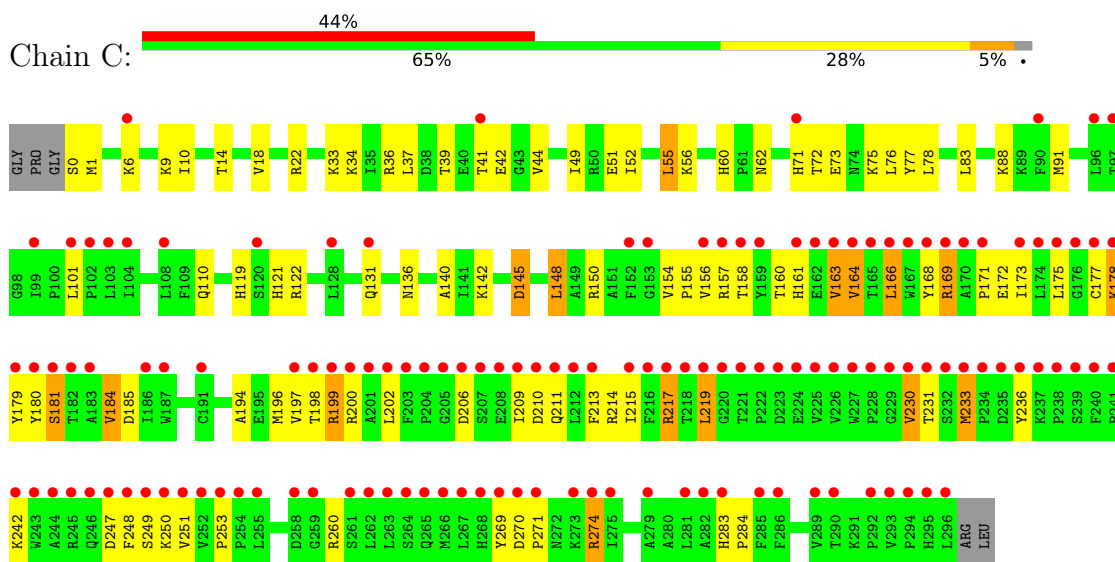
3 Residue-property plots

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

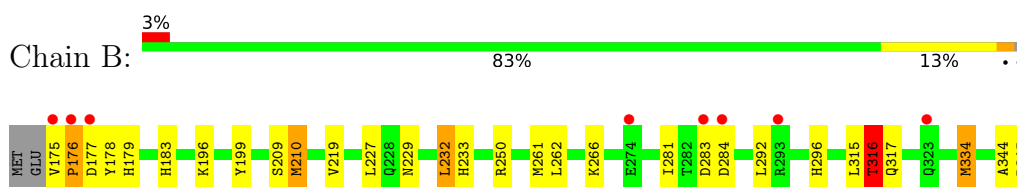
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 1: CELL DIVISION PROTEIN KINASE 2

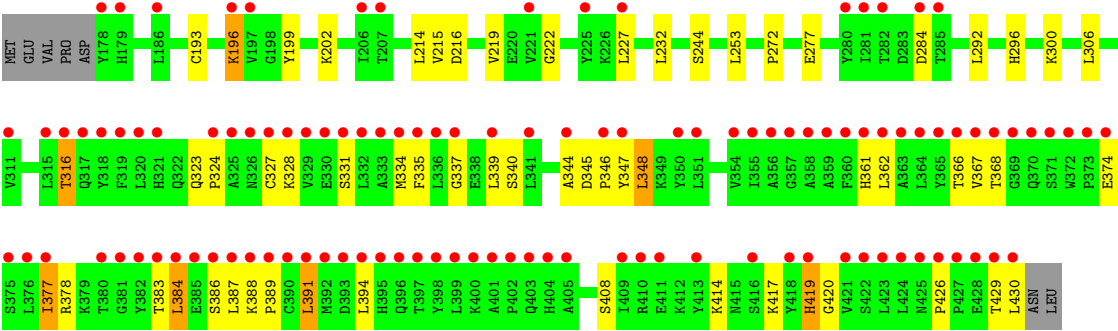


• Molecule 2: CYCLIN A2





● 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	74.12Å 134.73Å 148.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.10 99.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (100.00-2.10) 98.6 (99.70-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.276 0.232 , 0.272	Depositor DCC
R_{free} test set	4305 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9318	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 4.08% 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, MG, SGM, N20

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	0.79	0/2451	0.98	5/3324 (0.2%)
1	C	0.62	0/2446	0.93	2/3319 (0.1%)
2	B	0.78	1/2147 (0.0%)	0.95	1/2915 (0.0%)
2	D	0.59	0/2094	0.91	2/2842 (0.1%)
All	All	0.70	1/9138 (0.0%)	0.94	10/12400 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	210	MET	SD-CE	-5.14	1.66	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CB-CA-C	-10.63	98.12	112.04
1	A	257	GLU	N-CA-C	5.75	117.22	111.07
1	C	253	PRO	N-CA-C	5.75	117.71	110.70
1	A	247	ASP	CB-CA-C	5.49	118.67	109.89
1	A	230	VAL	N-CA-CB	5.39	117.21	110.47
1	C	230	VAL	CB-CA-C	-5.31	105.08	112.04
2	B	316	THR	N-CA-CB	-5.13	102.58	110.12
2	D	426	PRO	O-C-N	5.11	123.66	121.31
2	D	272	PRO	O-C-N	5.07	123.53	121.15
1	A	253	PRO	N-CA-C	5.05	116.86	110.70

There are no chirality outliers.

There are no planarity outliers.

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	2388	0	2428	45	1
1	C	2392	0	2432	57	0
2	B	2089	0	2112	34	1
2	D	2045	0	2070	35	0
3	A	25	0	20	3	0
3	C	25	0	20	2	0
4	B	6	0	7	0	0
4	D	6	0	8	1	0
5	B	1	0	0	0	0
6	A	144	0	0	6	0
6	B	132	0	0	8	0
6	C	41	0	0	4	0
6	D	24	0	0	0	0
All	All	9318	0	9097	164	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 9.

All (164) 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:B:210:MET:HE1	2:B:250:ARG:HB2	1.28	1.08
2:B:210:MET:HE1	2:B:250:ARG:CB	1.94	0.95
2:B:210:MET:CE	2:B:250:ARG:HB2	2.07	0.84
1:A:60:HIS:HD2	1:A:62:ASN:H	1.26	0.84
1:A:227:TRP:O	1:A:230:VAL:HG22	1.84	0.77
1:C:39:THR:HG21	6:C:2023:HOH:O	1.85	0.77
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.66	0.76
1:A:60:HIS:CD2	1:A:62:ASN:H	2.02	0.76
1:C:177:CYS:HB2	1:C:233:MET:HE3	1.68	0.74
2:B:177:ASP:OD2	6:B:2015:HOH:O	2.05	0.74
2:B:315:LEU:CD1	2:B:334[A]:MET:HE3	2.16	0.74
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.23	0.74
1:A:154:VAL:O	2:B:316:THR:HG23	1.91	0.70
1:C:60:HIS:HD2	1:C:62:ASN:H	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.60	0.70
2:B:315:LEU:HD12	2:B:334[A]:MET:CE	2.23	0.69
2:B:315:LEU:HD13	2:B:334[A]:MET:HE3	1.74	0.69
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.29	0.68
1:C:60:HIS:CD2	1:C:62:ASN:H	2.12	0.68
1:C:168:TYR:O	6:C:2036:HOH:O	2.13	0.67
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.77	0.67
1:A:154:VAL:O	2:B:316:THR:CG2	2.43	0.66
1:A:295:HIS:ND1	1:A:295:HIS:N	2.43	0.66
2:B:229:ASN:HD22	2:B:334[B]:MET:HE2	1.63	0.64
2:D:193:CYS:SG	4:D:1193:SGM:S1	2.55	0.64
1:A:161:HIS:HD2	6:A:2087:HOH:O	1.81	0.63
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.34	0.63
1:A:89:LYS:HD2	6:A:2144:HOH:O	1.98	0.62
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.81	0.62
2:B:227:LEU:HD12	2:B:261:MET:HE3	1.82	0.62
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.81	0.61
1:C:83:LEU:HD11	1:C:142:LYS:HD2	1.83	0.61
1:C:177:CYS:C	1:C:179:TYR:H	2.09	0.60
2:B:315:LEU:CD1	2:B:334[A]:MET:CE	2.78	0.59
1:A:74:ASN:N	1:A:74:ASN:OD1	2.35	0.59
1:A:137:THR:O	1:A:293:VAL:HG13	2.02	0.59
1:C:156:VAL:HG21	1:C:180:TYR:O	2.02	0.58
1:A:177:CYS:SG	1:A:179:TYR:O	2.53	0.58
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.33	0.58
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.85	0.58
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.67	0.58
1:C:177:CYS:C	1:C:179:TYR:N	2.61	0.58
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.92	0.58
1:C:260:ARG:HD3	6:C:2039:HOH:O	2.03	0.57
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.87	0.56
2:B:175:VAL:N	2:B:179:HIS:HE1	2.02	0.56
1:C:213:PHE:O	1:C:217:ARG:HB2	2.04	0.56
2:B:395:HIS:HE1	2:B:427:PRO:O	1.89	0.56
1:C:172:GLU:CD	1:C:274:ARG:HH22	2.13	0.55
1:C:219:LEU:HB2	1:C:269:TYR:HE2	1.72	0.55
2:B:315:LEU:HD12	2:B:334[A]:MET:HE3	1.86	0.55
2:D:337:GLY:O	2:D:340:SER:OG	2.23	0.55
1:A:39:THR:C	1:A:41:THR:H	2.15	0.55
1:C:177:CYS:O	1:C:179:TYR:N	2.40	0.55
2:D:347:TYR:OH	2:D:394:LEU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.88	0.54
2:B:175:VAL:O	6:B:2012:HOH:O	2.19	0.54
1:C:51:GLU:O	1:C:55:LEU:HB2	2.07	0.54
1:C:88:LYS:HE3	1:C:131:GLN:NE2	2.23	0.54
1:C:88:LYS:HB2	1:C:131:GLN:HE21	1.73	0.53
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.89	0.53
2:B:316:THR:HG21	6:B:2005:HOH:O	2.08	0.53
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.45	0.52
1:A:64:VAL:HG21	3:A:1298:N20:C8	2.40	0.52
2:D:383:THR:O	2:D:386:SER:N	2.42	0.52
1:A:126:ARG:HB3	1:A:163:VAL:HG22	1.91	0.52
1:C:219:LEU:HB2	1:C:269:TYR:CE2	2.45	0.52
1:A:95:ALA:HA	6:A:2044:HOH:O	2.11	0.51
1:A:197:VAL:HG11	1:A:252:VAL:HG12	1.93	0.51
1:C:72:THR:HG22	1:C:73:GLU:N	2.26	0.51
3:A:1298:N20:N1	3:A:1298:N20:H18	2.26	0.50
2:B:233:HIS:HE1	6:B:2089:HOH:O	1.93	0.50
1:A:119:HIS:HD2	6:B:2016:HOH:O	1.94	0.50
1:C:83:LEU:HD23	1:C:136:ASN:HB3	1.94	0.49
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.47	0.49
1:A:5:GLN:HB2	1:A:24:LYS:HE2	1.94	0.49
1:C:181:SER:O	1:C:184:VAL:HG13	2.12	0.49
2:D:374:GLU:HA	2:D:377:ILE:HG13	1.94	0.48
1:A:126:ARG:HB3	1:A:163:VAL:CG2	2.43	0.48
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.48	0.48
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.77	0.48
1:C:154:VAL:O	2:D:316:THR:HB	2.13	0.48
1:A:119:HIS:CD2	1:A:182:THR:HB	2.48	0.48
2:B:175:VAL:O	2:B:177:ASP:N	2.46	0.48
1:C:110:GLN:OE1	1:C:140:ALA:HA	2.13	0.48
2:B:296:HIS:CD2	6:B:2067:HOH:O	2.66	0.48
2:D:216:ASP:OD2	2:D:408:SER:HB2	2.13	0.48
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.96	0.48
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.95	0.48
1:A:72:THR:HG22	1:A:73:GLU:H	1.79	0.47
1:C:71:HIS:CE1	2:D:296:HIS:NE2	2.82	0.47
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.95	0.47
1:C:42:GLU:HB3	6:C:2013:HOH:O	2.13	0.47
2:D:419:HIS:ND1	2:D:419:HIS:N	2.62	0.47
1:A:51:GLU:O	1:A:55:LEU:HB2	2.15	0.47
2:B:175:VAL:N	2:B:179:HIS:CE1	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:367:VAL:HG12	2:D:368:THR:HG23	1.96	0.47
1:C:121:HIS:C	1:C:122:ARG:HG3	2.40	0.46
1:C:175:LEU:HB2	1:C:233:MET:HE2	1.97	0.46
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.97	0.46
1:C:10:ILE:HD12	1:C:18:VAL:HG12	1.97	0.46
1:C:270:ASP:O	1:C:271:PRO:C	2.58	0.46
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.51	0.46
2:B:296:HIS:NE2	6:B:2065:HOH:O	2.36	0.46
1:C:88:LYS:HA	1:C:91:MET:HE2	1.98	0.46
3:C:1298:N20:N1	3:C:1298:N20:C18	2.78	0.46
1:A:85:GLN:HE21	1:A:90:PHE:HB2	1.81	0.45
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.51	0.45
2:B:210:MET:HE1	2:B:250:ARG:HB3	1.90	0.45
1:C:62:ASN:HA	1:C:142:LYS:HG2	1.98	0.45
2:D:196:LYS:HB3	2:D:244:SER:HB3	1.99	0.45
2:D:386:SER:C	2:D:388:LYS:H	2.24	0.45
2:B:176:PRO:HA	2:B:179:HIS:CG	2.52	0.45
1:C:211:GLN:O	1:C:215:ILE:HG12	2.17	0.45
1:A:126:ARG:HD2	1:A:163:VAL:HG21	1.99	0.44
2:B:345:ASP:HA	2:B:346:PRO:HA	1.74	0.44
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.00	0.44
1:C:194:ALA:CB	1:C:202:LEU:HD22	2.48	0.44
1:C:248:PHE:HA	1:C:251:VAL:HG23	2.00	0.44
1:A:7:VAL:HG12	1:A:8:GLU:HG2	1.99	0.44
1:C:88:LYS:HE3	1:C:131:GLN:CD	2.42	0.44
1:C:161:HIS:CD2	1:C:173:ILE:HG22	2.53	0.44
1:C:231:THR:HA	1:C:236:TYR:CD1	2.52	0.44
1:A:268:HIS:CD2	6:A:2130:HOH:O	2.70	0.44
2:B:183:HIS:HB2	2:B:317:GLN:NE2	2.32	0.44
1:C:71:HIS:CE1	2:D:296:HIS:CD2	3.06	0.43
2:D:344:ALA:O	2:D:348:LEU:HB2	2.18	0.43
1:A:260:ARG:HD3	6:A:2123:HOH:O	2.17	0.43
3:A:1298:N20:N1	3:A:1298:N20:C18	2.79	0.43
1:A:293:VAL:HG13	1:A:294:PRO:HD2	2.01	0.43
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.99	0.43
1:C:166:LEU:HA	1:C:169:ARG:HH21	1.83	0.43
1:C:210:ASP:O	1:C:214:ARG:HG3	2.18	0.43
1:A:177:CYS:HB2	1:A:233:MET:CE	2.48	0.43
1:C:37:LEU:HD22	1:C:44:VAL:HG22	2.00	0.43
1:C:161:HIS:HD2	1:C:173:ILE:HG22	1.83	0.43
3:C:1298:N20:N1	3:C:1298:N20:H18	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:VAL:O	2:D:219:VAL:HG23	2.18	0.43
2:D:323:GLN:HA	2:D:323:GLN:OE1	2.19	0.43
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.54	0.43
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.54	0.43
1:C:14:THR:HG23	1:C:145:ASP:OD2	2.19	0.43
1:C:71:HIS:NE2	2:D:296:HIS:NE2	2.67	0.43
1:A:91:MET:HG2	1:A:99:ILE:HD11	2.01	0.42
1:A:60:HIS:HD2	1:A:62:ASN:N	2.07	0.42
1:A:154:VAL:HA	1:A:155:PRO:HA	1.86	0.42
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.54	0.42
6:A:2039:HOH:O	2:D:202:LYS:HE2	2.20	0.42
2:D:196:LYS:HG2	2:D:199:TYR:HB3	2.01	0.42
2:D:323:GLN:HA	2:D:324:PRO:HA	1.76	0.42
2:D:327:CYS:HB3	2:D:419:HIS:CD2	2.54	0.42
1:C:169:ARG:HE	1:C:169:ARG:HB2	1.59	0.41
2:D:345:ASP:HA	2:D:346:PRO:HA	1.76	0.41
1:A:41:THR:HB	1:A:42:GLU:H	1.60	0.41
1:A:217:ARG:HG2	1:A:243:TRP:CE2	2.55	0.41
2:D:214:LEU:HD22	2:D:253:LEU:HG	2.03	0.41
1:C:1:MET:HE2	1:C:77:TYR:CD1	2.56	0.41
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.56	0.41
1:C:148:LEU:HD12	1:C:148:LEU:HA	1.86	0.41
1:A:119:HIS:HE1	1:A:185:ASP:OD2	2.04	0.41
2:B:178:TYR:N	6:B:2012:HOH:O	2.23	0.41
1:C:198:THR:O	1:C:199:ARG:HB2	2.21	0.41
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.56	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)
1:A:199:ARG:NH2	2:B:374:GLU:OE2[4_456]	2.07	0.13

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%)	283 (96%)	9 (3%)	2 (1%)	18	15
1	C	295/302 (98%)	270 (92%)	19 (6%)	6 (2%)	6	2
2	B	258/260 (99%)	254 (98%)	3 (1%)	1 (0%)	30	28
2	D	251/260 (96%)	236 (94%)	13 (5%)	2 (1%)	16	12
All	All	1098/1124 (98%)	1043 (95%)	44 (4%)	11 (1%)	12	9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	176	PRO
1	C	164	VAL
1	C	166	LEU
1	C	178	LYS
1	A	40	GLU
1	A	164	VAL
1	C	145	ASP
2	D	387	LEU
1	C	199	ARG
2	D	384	LEU
1	C	171	PRO

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%)	238 (90%)	25 (10%)	8	5
1	C	262/264 (99%)	227 (87%)	35 (13%)	4	2
2	B	234/234 (100%)	217 (93%)	17 (7%)	13	10
2	D	227/234 (97%)	206 (91%)	21 (9%)	8	6
All	All	986/996 (99%)	888 (90%)	98 (10%)	7	5

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	6	LYS
1	A	34	LYS
1	A	39	THR
1	A	40	GLU
1	A	41	THR
1	A	55	LEU
1	A	73	GLU
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	83	LEU
1	A	97	THR
1	A	101	LEU
1	A	150	ARG
1	A	178	LYS
1	A	189	LEU
1	A	200	ARG
1	A	206	ASP
1	A	230	VAL
1	A	247	ASP
1	A	255	LEU
1	A	273	LYS
1	A	295	HIS
1	A	296	LEU
2	B	196	LYS
2	B	209	SER
2	B	232	LEU
2	B	281	ILE
2	B	283	ASP
2	B	284	ASP
2	B	292	LEU
2	B	316	THR
2	B	334[A]	MET
2	B	334[B]	MET
2	B	348	LEU
2	B	371	SER
2	B	384	LEU
2	B	391	LEU
2	B	392	MET
2	B	417	LYS
2	B	428	GLU

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Mol	Chain	Res	Type
1	C	0	SER
1	C	6	LYS
1	C	9	LYS
1	C	22	ARG
1	C	33	LYS
1	C	34	LYS
1	C	36	ARG
1	C	41	THR
1	C	55	LEU
1	C	56	LYS
1	C	75	LYS
1	C	101	LEU
1	C	148	LEU
1	C	150	ARG
1	C	157	ARG
1	C	158	THR
1	C	163	VAL
1	C	169	ARG
1	C	178	LYS
1	C	181	SER
1	C	184	VAL
1	C	196	MET
1	C	197	VAL
1	C	200	ARG
1	C	206	ASP
1	C	209	ILE
1	C	217	ARG
1	C	219	LEU
1	C	230	VAL
1	C	233	MET
1	C	242	LYS
1	C	247	ASP
1	C	249	SER
1	C	250	LYS
1	C	274	ARG
2	D	196	LYS
2	D	232	LEU
2	D	277	GLU
2	D	284	ASP
2	D	292	LEU
2	D	300	LYS
2	D	316	THR

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Mol	Chain	Res	Type
2	D	328	LYS
2	D	331	SER
2	D	334	MET
2	D	348	LEU
2	D	362	LEU
2	D	366	THR
2	D	377	ILE
2	D	378	ARG
2	D	384	LEU
2	D	391	LEU
2	D	417	LYS
2	D	419	HIS
2	D	429	THR
2	D	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	85	GLN
1	A	119	HIS
1	A	161	HIS
1	A	265	GLN
1	A	268	HIS
2	B	179	HIS
2	B	229	ASN
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	313	GLN
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
2	B	431	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	119	HIS
1	C	131	GLN
1	C	161	HIS

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Mol	Chain	Res	Type
1	C	268	HIS
2	D	183	HIS
2	D	254	GLN
2	D	296	HIS
2	D	361	HIS
2	D	396	GLN
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	1.44	1 (12%)	10,14,16	0.97	0
1	TPO	C	160	1	8,10,11	1.27	1 (12%)	10,14,16	0.82	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	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O1P	3.45	1.61	1.50
1	C	160	TPO	P-O1P	2.66	1.58	1.50

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 5 ligands modelled in this entry, 1 is 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	N20	C	1298	-	28,28,28	1.23	3 (10%)	37,38,38	1.82	8 (21%)
4	SGM	B	1193	-	5,5,5	0.68	0	5,5,5	0.49	0
3	N20	A	1298	-	28,28,28	1.47	7 (25%)	37,38,38	2.07	7 (18%)
4	SGM	D	1193	-	5,5,5	0.32	0	5,5,5	0.62	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	N20	C	1298	-	-	0/9/17/17	0/4/4/4
4	SGM	B	1193	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N20	A	1298	-	-	0/9/17/17	0/4/4/4
4	SGM	D	1193	-	-	3/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	N20	C8-N7	3.81	1.40	1.32
3	C	1298	N20	C5-C6	3.24	1.47	1.41
3	C	1298	N20	C8-N7	3.06	1.38	1.32
3	A	1298	N20	C5-C4	2.94	1.43	1.39
3	A	1298	N20	C5-C6	2.82	1.46	1.41
3	C	1298	N20	C5-C4	2.36	1.42	1.39
3	A	1298	N20	C17-N2	-2.24	1.35	1.40
3	A	1298	N20	C6-N1	2.07	1.35	1.32
3	A	1298	N20	C4-N9	2.06	1.39	1.36
3	A	1298	N20	C8-N9	2.02	1.40	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	N20	C4-N9-C8	-6.18	100.67	106.43
3	A	1298	N20	C5-C4-N3	-5.05	121.60	126.55
3	C	1298	N20	C5-C4-N3	-4.64	122.00	126.55
3	A	1298	N20	C2-N1-C6	4.47	123.08	115.38
3	A	1298	N20	C5-C6-N1	-4.46	117.53	123.49
3	C	1298	N20	C2-N1-C6	4.30	122.79	115.38
3	C	1298	N20	C4-N9-C8	-4.15	102.57	106.43
3	A	1298	N20	C5-C4-N9	3.90	110.88	105.67
3	C	1298	N20	C5-C6-N1	-3.62	118.64	123.49
3	C	1298	N20	N3-C2-N1	-3.32	120.82	126.26
3	C	1298	N20	C5-C4-N9	3.30	110.08	105.67
3	A	1298	N20	N3-C2-N1	-2.86	121.58	126.26
3	A	1298	N20	O6-C6-C5	2.81	120.44	116.73
3	C	1298	N20	O6-C6-C5	2.42	119.93	116.73
3	C	1298	N20	C17-N2-C2	-2.20	123.44	129.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1193	SGM	O2-C2-C3-O3

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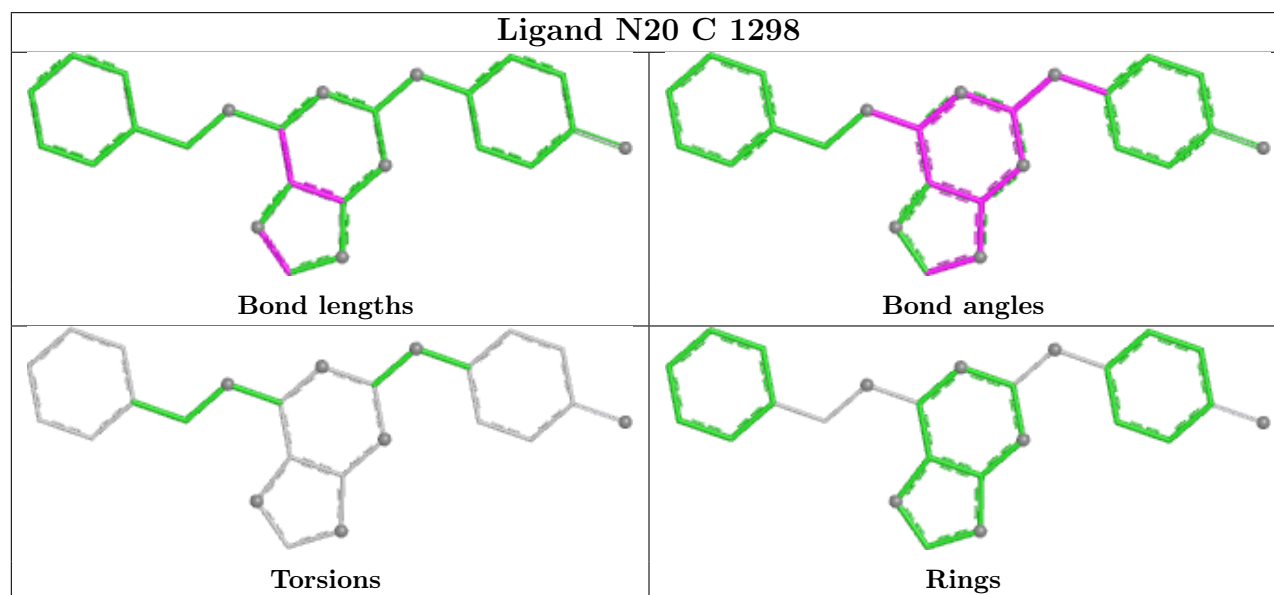
Mol	Chain	Res	Type	Atoms
4	D	1193	SGM	C1-C2-C3-O3
4	B	1193	SGM	S1-C1-C2-O2
4	D	1193	SGM	S1-C1-C2-O2

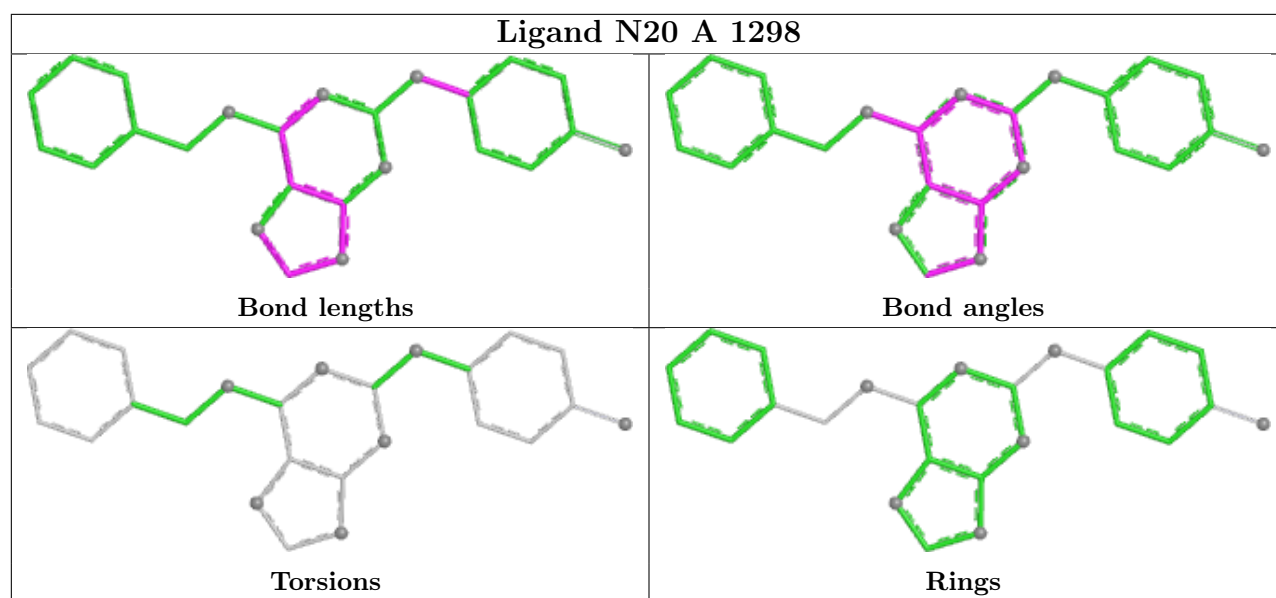
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1298	N20	2	0
3	A	1298	N20	3	0
4	D	1193	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	295/302 (97%)	0.08	17 (5%) 29 30	11, 21, 45, 62	3 (1%)
1	C	296/302 (98%)	1.98	133 (44%) 0 1	23, 46, 75, 79	1 (0%)
2	B	258/260 (99%)	0.05	9 (3%) 47 49	11, 23, 41, 53	2 (0%)
2	D	253/260 (97%)	1.93	111 (43%) 0 1	21, 49, 70, 76	0
All	All	1102/1124 (98%)	1.01	270 (24%) 2 2	11, 33, 69, 79	6 (0%)

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	ILE	8.3
2	B	175	VAL	7.8
1	C	174	LEU	7.4
2	D	372	TRP	6.5
1	C	243	TRP	6.2
2	D	384	LEU	5.9
2	D	325	ALA	5.8
1	C	230	VAL	5.5
2	D	430	LEU	5.4
1	C	180	TYR	5.4
1	C	226	VAL	5.4
1	C	209	ILE	5.4
1	C	215	ILE	5.4
1	C	253	PRO	5.3
1	C	170	ALA	5.3
2	D	356	ALA	5.3
1	C	166	LEU	5.2
1	A	296	LEU	5.0
1	C	225	VAL	5.0
2	D	395	HIS	5.0
1	C	216	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	229	GLY	5.0
2	D	429	THR	4.9
1	C	234	PRO	4.8
1	C	254	PRO	4.7
1	C	175	LEU	4.7
1	C	248	PHE	4.7
2	D	376	LEU	4.7
2	D	364	LEU	4.6
1	C	71	HIS	4.6
1	C	241	PRO	4.6
1	C	271	PRO	4.6
1	C	159	TYR	4.6
2	D	373	PRO	4.6
1	C	252	VAL	4.5
1	A	39	THR	4.5
1	C	219	LEU	4.5
2	D	332	LEU	4.5
1	C	228	PRO	4.5
1	C	296	LEU	4.5
1	C	187	TRP	4.5
2	D	369	GLY	4.5
1	C	227	TRP	4.4
1	A	72	THR	4.4
1	C	213	PHE	4.4
2	D	360	PHE	4.4
2	D	363	ALA	4.4
2	D	402	PRO	4.3
2	D	367	VAL	4.3
1	C	204	PRO	4.3
1	C	203	PHE	4.2
2	B	177	ASP	4.2
1	C	255	LEU	4.2
2	D	423	LEU	4.2
1	C	165	THR	4.2
2	D	426	PRO	4.2
2	D	413	TYR	4.2
1	C	233	MET	4.2
2	D	391	LEU	4.2
1	A	40	GLU	4.2
1	C	269	TYR	4.2
2	D	362	LEU	4.1
1	C	101	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	176	PRO	4.0
2	D	390	CYS	4.0
1	A	71	HIS	4.0
1	C	99	ILE	4.0
2	D	418	TYR	4.0
2	D	387	LEU	3.9
1	C	164	VAL	3.9
2	D	366	THR	3.9
2	D	354	VAL	3.9
1	C	104	ILE	3.8
1	C	201	ALA	3.8
2	D	346	PRO	3.8
1	C	238	PRO	3.8
1	C	250	LYS	3.8
1	C	251	VAL	3.8
2	D	334	MET	3.7
2	D	350	TYR	3.7
1	C	198	THR	3.7
1	C	169	ARG	3.7
2	D	320	LEU	3.7
1	C	240	PHE	3.7
2	D	347	TYR	3.7
1	C	295	HIS	3.6
1	C	224	GLU	3.6
1	C	202	LEU	3.6
1	C	212	LEU	3.6
2	D	399	LEU	3.6
2	D	424	LEU	3.6
1	C	242	LYS	3.6
2	D	389	PRO	3.6
2	D	409	ILE	3.6
1	C	96	LEU	3.6
1	C	200	ARG	3.6
1	C	179	TYR	3.6
2	D	382	TYR	3.6
2	D	392	MET	3.5
1	C	236	TYR	3.5
2	D	405	ALA	3.5
2	D	280	TYR	3.5
2	D	394	LEU	3.5
2	D	351	LEU	3.4
2	D	403	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	419	HIS	3.4
2	D	368	THR	3.4
2	D	377	ILE	3.4
1	C	262	LEU	3.4
2	D	365	TYR	3.4
1	C	249	SER	3.4
2	D	375	SER	3.4
1	A	96	LEU	3.4
2	D	339	LEU	3.4
2	B	284	ASP	3.3
2	D	358	ALA	3.3
1	C	177	CYS	3.3
1	C	171	PRO	3.3
1	C	292	PRO	3.3
2	D	329	VAL	3.3
1	C	267	LEU	3.3
2	D	428	GLU	3.3
1	A	295	HIS	3.2
1	C	244	ALA	3.2
2	D	401	ALA	3.2
1	C	246	GLN	3.2
1	A	97	THR	3.2
2	D	333	ALA	3.1
1	C	205	GLY	3.1
1	C	231	THR	3.1
2	D	388	LYS	3.1
2	D	327	CYS	3.1
1	C	156	VAL	3.1
1	C	197	VAL	3.1
1	C	268	HIS	3.1
1	A	41	THR	3.1
1	C	221	THR	3.1
1	C	217	ARG	3.1
1	C	167	TRP	3.0
1	C	218	THR	3.0
1	C	247	ASP	3.0
2	D	284	ASP	3.0
1	C	263	LEU	3.0
1	C	222	PRO	3.0
2	D	324	PRO	3.0
2	D	315	LEU	3.0
2	D	359	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	410	ARG	3.0
2	D	281	ILE	3.0
2	D	397	THR	3.0
1	C	258	ASP	3.0
1	C	294	PRO	3.0
2	D	398	TYR	3.0
1	A	73	GLU	2.9
1	C	178	LYS	2.9
1	C	286	PHE	2.9
2	D	331	SER	2.9
1	C	223	ASP	2.9
1	C	158	THR	2.9
2	D	311	VAL	2.9
2	D	317	GLN	2.9
2	D	427	PRO	2.9
2	D	318	TYR	2.9
2	D	380	THR	2.8
1	C	97	THR	2.8
1	C	289	VAL	2.8
1	C	152	PHE	2.8
2	D	355	ILE	2.8
1	C	239	SER	2.8
2	D	416	SER	2.8
2	D	319	PHE	2.8
2	D	344	ALA	2.8
1	C	102	PRO	2.8
2	D	421	VAL	2.8
2	D	422	SER	2.7
2	D	335	PHE	2.7
2	D	383	THR	2.7
1	C	163	VAL	2.7
1	C	275	ILE	2.7
2	D	326	ASN	2.7
1	C	232	SER	2.7
1	C	266	MET	2.7
1	C	90	PHE	2.7
1	C	285	PHE	2.7
1	C	168	TYR	2.7
2	D	385	GLU	2.7
2	D	225	TYR	2.7
2	D	361	HIS	2.7
1	A	74	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	161	HIS	2.6
1	C	6	LYS	2.6
1	C	210	ASP	2.6
2	D	386	SER	2.6
1	C	220	GLY	2.6
1	C	259	GLY	2.6
2	D	321	HIS	2.6
1	C	273	LYS	2.6
2	D	400	LYS	2.6
2	D	371	SER	2.6
1	C	199	ARG	2.6
1	C	207	SER	2.6
1	C	264	SER	2.6
2	D	374	GLU	2.5
2	D	178	TYR	2.5
1	C	211	GLN	2.5
1	C	281	LEU	2.5
1	C	293	VAL	2.5
1	C	120	SER	2.5
1	C	237	LYS	2.5
2	D	227	LEU	2.5
1	C	274	ARG	2.5
1	C	153	GLY	2.5
2	B	432	LEU	2.4
2	D	381	GLY	2.4
1	C	208	GLU	2.4
1	C	265	GLN	2.4
1	A	36	ARG	2.4
2	D	196	LYS	2.4
2	B	323	GLN	2.4
2	D	357	GLY	2.4
1	C	235	ASP	2.4
2	D	328	LYS	2.4
1	C	128	LEU	2.3
2	D	341	LEU	2.3
1	C	157	ARG	2.3
1	C	176	GLY	2.3
2	D	206	ILE	2.3
2	D	396	GLN	2.3
1	C	282	ALA	2.3
1	C	103	LEU	2.3
1	C	162	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	270	ASP	2.2
2	B	283	ASP	2.2
2	D	337	GLY	2.2
2	D	404	HIS	2.2
1	C	41	THR	2.2
1	C	186	ILE	2.2
2	D	285	THR	2.2
1	C	279	ALA	2.2
2	D	330	GLU	2.2
2	D	186	LEU	2.2
1	A	179	TYR	2.2
1	C	245	ARG	2.2
2	D	425	ASN	2.2
2	D	207	THR	2.2
2	D	370	GLN	2.2
2	D	336	LEU	2.2
2	D	197	VAL	2.1
1	C	183	ALA	2.1
2	D	179	HIS	2.1
1	C	181	SER	2.1
1	C	261	SER	2.1
2	D	393	ASP	2.1
1	C	182	THR	2.1
2	B	274	GLU	2.1
2	D	411	GLU	2.1
1	C	283	HIS	2.1
1	C	290	THR	2.1
2	B	293	ARG	2.1
1	A	0	SER	2.1
1	C	131	GLN	2.0
1	C	206	ASP	2.0
1	A	161	HIS	2.0
1	A	2	GLU	2.0
2	D	221	VAL	2.0
1	A	95	ALA	2.0
1	C	108	LEU	2.0
1	C	191	CYS	2.0
2	D	282	THR	2.0
2	D	316	THR	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	0.90	0.13	39,48,51,52	0
1	TPO	A	160	11/12	0.98	0.05	14,18,19,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

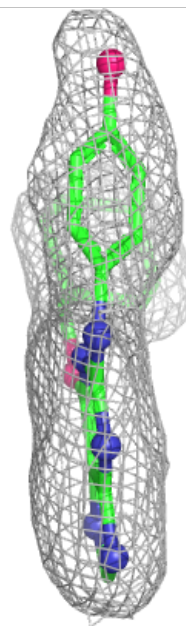
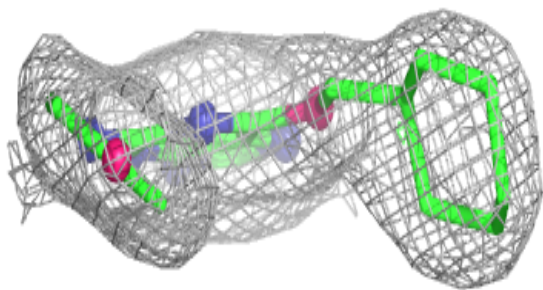
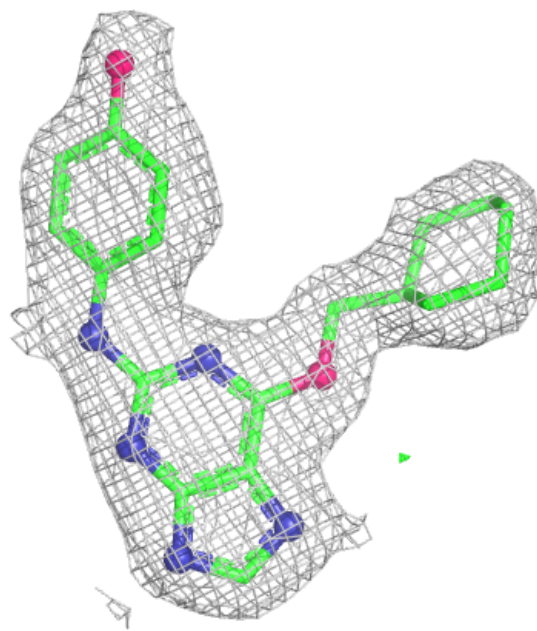
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SGM	D	1193	6/6	0.86	0.15	51,54,55,55	0
4	SGM	B	1193	6/6	0.92	0.14	34,38,41,47	0
3	N20	C	1298	25/25	0.93	0.10	29,35,38,42	0
3	N20	A	1298	25/25	0.94	0.08	24,26,29,30	0
5	MG	B	1433	1/1	0.98	0.04	35,35,35,35	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.

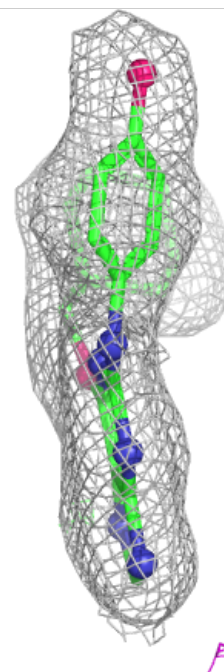
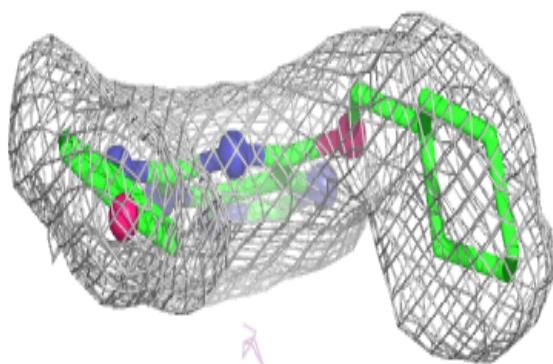
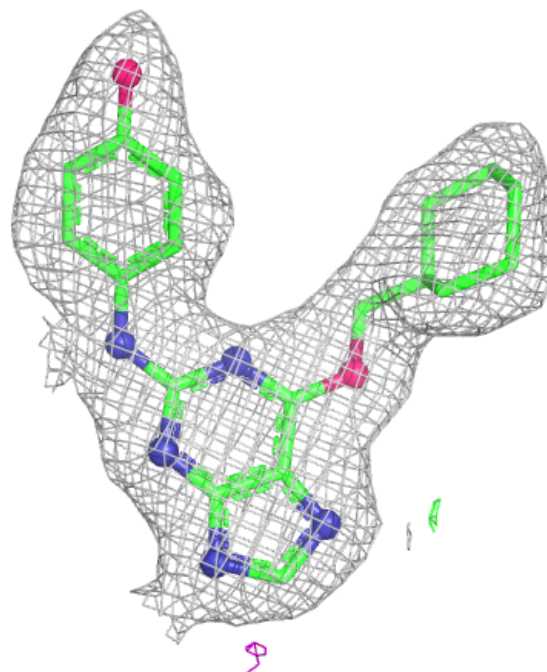
Electron density around N20 C 1298:

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



Electron density around N20 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 ⓘ

There are no such residues in this entry.