Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 07:15 pm GMT

PDB ID	:	4CFN
Title	:	Structure-based design of C8-substituted O6-cyclohexylmethoxyguanine CDK1 and 2 inhibitors.
Authors	:	Carbain, B.; Paterson, D.J.; Anscombe, E.; Campbell, A.; Cano, C.; Echalier, A.; Endicott, J.; Golding, B.T.; Haggerty, K.; Hardcastle, I.R.; Jewsbury, P.; Newell, D.R.; Noble, M.E.M.; Roche, C.; Wang, L.Z.; Griffin, R.
Deposited on	:	2013-11-19
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

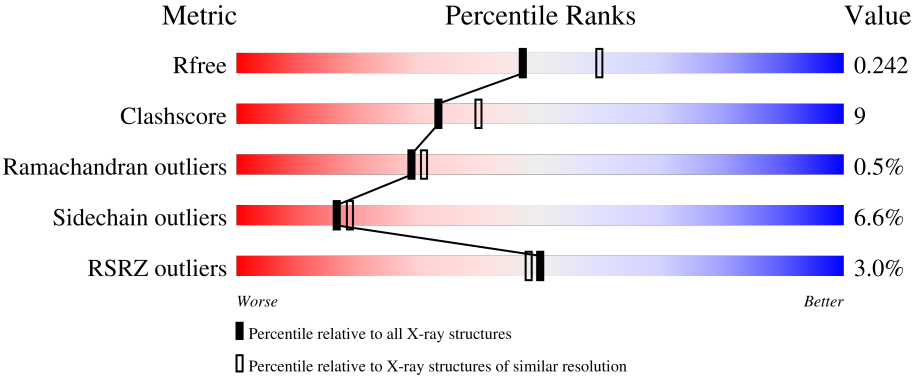
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	4% 78% 17% • • •
1	C	302	2% 80% 15% • •
2	B	258	83% 14% • • •
2	D	258	5% 83% 14% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JYM	A	1298	-	-	X	-
4	DTT	D	1433	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9533 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYCLIN-DEPENDENT KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	297	2405	1561	412	423	1	8	0	2	0
1	C	297	2400	1556	407	428	1	8	0	2	0

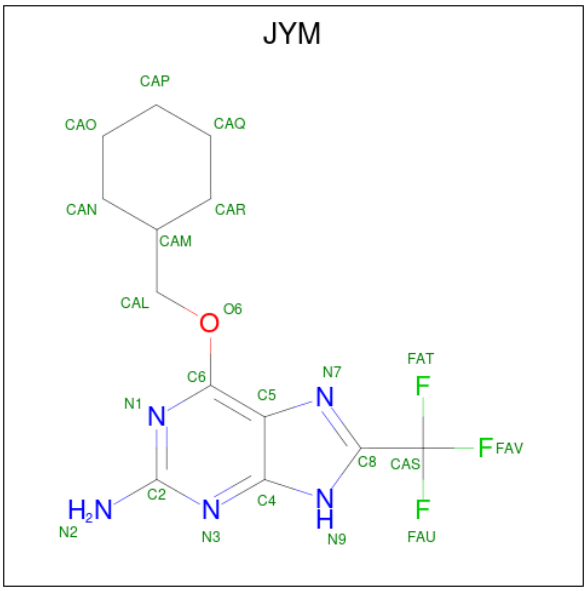
There are 8 discrepancies between the modelled and reference sequences:

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
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

- Molecule 2 is a protein called CYCLIN-A2.

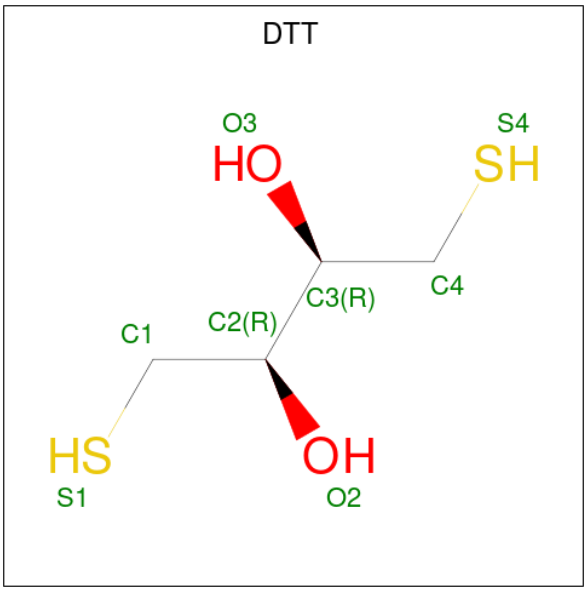
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	254	2053	1332	335	375	11	0	0	0
2	D	255	2060	1337	336	376	11	0	0	0

- Molecule 3 is 6-(cyclohexylmethoxy)-8-(trifluoromethyl)-9H-purin-2-amine (three-letter code: JYM) (formula: $C_{13}H_{16}F_3N_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	22	13	3	5	1	0	0
			Total	C	F	N	O		
3	C	1	22	13	3	5	1	0	0

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	B	1	8	4	2	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	D	1	8	4	2	2	0	0

- Molecule 5 is water.

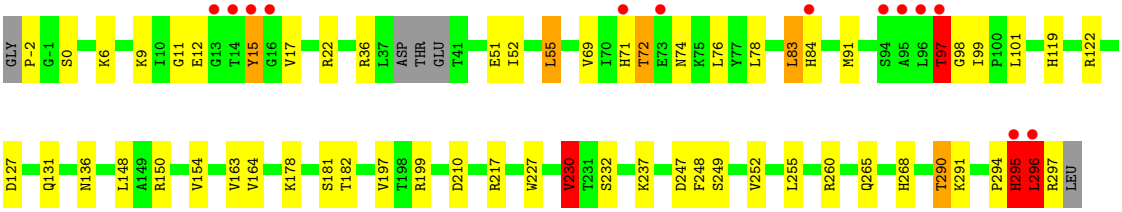
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	192	192	192	0	0
			Total	O		
5	B	151	151	151	0	0
			Total	O		
5	C	123	123	123	0	0
			Total	O		
5	D	89	89	89	0	0

3 Residue-property plots (i)

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

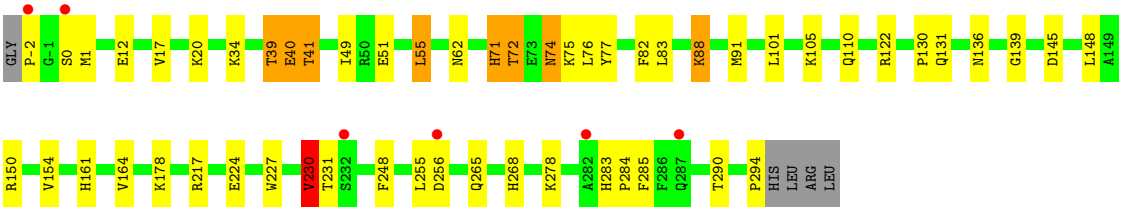
• Molecule 1: CYCLIN-DEPENDENT KINASE 2

Chain A:



• Molecule 1: CYCLIN-DEPENDENT KINASE 2

Chain C:

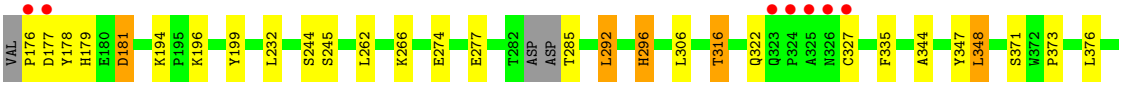


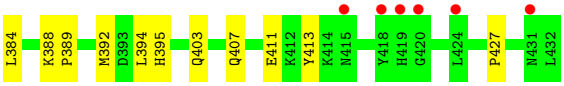
• Molecule 2: CYCLIN-A2

Chain B:

• Molecule 2: CYCLIN-A2

Chain D:




L384
K388
P389
M392
D393
L394
H395
Q403
Q407
E411
K412
Y413
K414
N415
Y418
H419
G420
L424
P427
N431
L432

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.98Å 134.42Å 147.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.50 – 2.20 52.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (99.50-2.20) 91.2 (52.30-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.197 , 0.241 0.200 , 0.242	Depositor DCC
R_{free} test set	3463 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9533	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 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DTT, JYM, TPO

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	0.87	0/2456	0.95	5/3329 (0.2%)
1	C	0.79	1/2451 (0.0%)	0.86	1/3325 (0.0%)
2	B	0.85	2/2101 (0.1%)	0.92	4/2850 (0.1%)
2	D	0.76	1/2109 (0.0%)	0.85	0/2861
All	All	0.82	4/9117 (0.0%)	0.90	10/12365 (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
1	A	0	3
1	C	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	277	GLU	CG-CD	6.74	1.62	1.51
2	B	277	GLU	CG-CD	5.34	1.59	1.51
2	B	431	ASN	CB-CG	5.09	1.62	1.51
1	C	40	GLU	C-O	5.06	1.32	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	327	CYS	CA-CB-SG	-11.29	93.68	114.00
1	A	217	ARG	NE-CZ-NH1	6.53	123.57	120.30
2	B	378	ARG	NE-CZ-NH1	5.84	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	423	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	C	230	VAL	CB-CA-C	-5.61	100.74	111.40
1	A	237	LYS	CD-CE-NZ	5.40	124.11	111.70
1	A	217	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	B	316	THR	N-CA-CB	-5.21	100.40	110.30
1	A	230	VAL	CB-CA-C	-5.18	101.55	111.40
1	A	127	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	294	PRO	Peptide
1	A	295	HIS	Peptide
1	A	97	THR	Peptide
1	C	39	THR	Peptide
1	C	71	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2405	0	2447	60	0
1	C	2400	0	2435	52	1
2	B	2053	0	2082	28	0
2	D	2060	0	2090	32	0
3	A	22	0	15	7	0
3	C	22	0	16	0	0
4	B	8	0	7	0	0
4	D	8	0	7	0	0
5	A	192	0	0	18	1
5	B	151	0	0	5	0
5	C	123	0	0	12	0
5	D	89	0	0	3	0
All	All	9533	0	9099	156	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 (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131[B]:GLN:NE2	3:A:1298:JYM:CAQ	1.72	1.48
1:A:131[B]:GLN:NE2	3:A:1298:JYM:CAR	1.90	1.32
1:C:72:THR:HB	5:C:2047:HOH:O	1.31	1.28
1:C:40:GLU:HA	1:C:41:THR:HG23	1.20	1.18
1:A:131[B]:GLN:NE2	3:A:1298:JYM:HAR2	1.53	1.13
1:A:131[B]:GLN:NE2	3:A:1298:JYM:HAQ1	1.72	1.04
1:C:40:GLU:HA	1:C:41:THR:CG2	1.93	0.97
1:A:131[B]:GLN:HE21	3:A:1298:JYM:HAR2	1.07	0.93
1:A:131[B]:GLN:HE21	3:A:1298:JYM:CAR	1.67	0.91
2:D:285:THR:N	5:D:2053:HOH:O	2.05	0.89
1:A:154:VAL:O	2:B:316:THR:HG23	1.72	0.88
1:C:41:THR:HG22	2:D:292:LEU:CD2	2.03	0.88
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.42	0.87
1:C:154:VAL:O	2:D:316:THR:HG23	1.75	0.86
2:B:431:ASN:OD1	2:B:431:ASN:O	1.95	0.85
1:A:15:TYR:HA	5:A:2009:HOH:O	1.78	0.83
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.96	0.83
1:C:72:THR:CB	5:C:2047:HOH:O	2.00	0.82
1:C:154:VAL:O	2:D:316:THR:CG2	2.28	0.82
1:C:39:THR:HG23	1:C:40:GLU:OE2	1.81	0.80
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.29	0.80
1:A:-2:PRO:HD2	5:A:2001:HOH:O	1.83	0.77
1:C:74:ASN:HB3	5:C:2049:HOH:O	1.83	0.76
1:A:268:HIS:ND1	5:A:2169:HOH:O	2.19	0.75
2:D:194:LYS:NZ	5:D:2007:HOH:O	2.19	0.75
1:A:268:HIS:HD2	5:A:2170:HOH:O	1.70	0.75
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.23	0.73
1:C:-2:PRO:HB2	5:C:2045:HOH:O	1.88	0.73
1:A:268:HIS:CD2	5:A:2170:HOH:O	2.42	0.71
1:A:295:HIS:HB2	1:A:296:LEU:HD23	1.72	0.70
1:A:97:THR:HB	1:A:98:GLY:O	1.92	0.70
1:A:268:HIS:CG	5:A:2169:HOH:O	2.45	0.70
1:A:119:HIS:HD2	5:A:2060:HOH:O	1.75	0.69
1:C:88:LYS:HG2	5:C:2054:HOH:O	1.91	0.68
1:C:71:HIS:CD2	2:D:296:HIS:HE1	2.11	0.68
1:A:154:VAL:O	2:B:316:THR:CG2	2.41	0.68
2:B:210:MET:HE1	2:B:250:ARG:CB	2.24	0.67
1:C:83:LEU:HD23	1:C:136:ASN:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:GLN:O	5:D:2063:HOH:O	2.11	0.67
2:B:210:MET:CE	2:B:250:ARG:HB2	2.24	0.67
5:A:2028:HOH:O	2:B:316:THR:HG21	1.93	0.67
1:C:40:GLU:HA	1:C:41:THR:CB	2.20	0.67
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.77	0.66
1:C:88:LYS:HA	1:C:91:MET:HE2	1.77	0.66
1:A:291:LYS:NZ	5:A:2185:HOH:O	2.29	0.66
1:A:72:THR:N	5:A:2038:HOH:O	2.29	0.65
2:B:285:THR:O	5:B:2076:HOH:O	2.15	0.64
1:C:41:THR:HG22	2:D:292:LEU:HD21	1.80	0.64
2:B:317:GLN:NE2	5:B:2005:HOH:O	2.14	0.62
1:A:295:HIS:CA	1:A:296:LEU:HB2	2.29	0.62
1:A:297:ARG:NH2	5:A:2045:HOH:O	2.33	0.61
1:A:9:LYS:HZ1	1:A:12:GLU:HG2	1.66	0.61
1:A:295:HIS:N	1:A:296:LEU:HB2	2.16	0.60
1:A:9:LYS:HZ3	1:A:17:VAL:HG13	1.66	0.60
1:C:41:THR:N	5:C:2026:HOH:O	2.34	0.59
1:A:15:TYR:CD1	1:A:15:TYR:N	2.71	0.59
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.84	0.58
1:A:9:LYS:NZ	1:A:11:GLY:C	2.57	0.58
1:A:98:GLY:HA2	1:A:199:ARG:NE	2.19	0.57
1:A:290:THR:OG1	1:A:291:LYS:N	2.37	0.57
1:A:72:THR:CA	5:A:2038:HOH:O	2.53	0.57
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.86	0.57
1:A:98:GLY:HA2	1:A:199:ARG:HE	1.70	0.56
1:A:227:TRP:O	1:A:230:VAL:HG22	2.06	0.56
1:C:278:LYS:NZ	2:D:181:ASP:OD2	2.35	0.56
1:C:40:GLU:CA	1:C:41:THR:OG1	2.54	0.56
2:B:395:HIS:HE1	2:B:427:PRO:O	1.89	0.55
2:B:417:LYS:HD3	2:B:418:TYR:CZ	2.42	0.55
5:C:2079:HOH:O	2:D:316:THR:HG21	2.05	0.55
1:A:71:HIS:CD2	2:B:296:HIS:CE1	2.94	0.55
1:C:268:HIS:HB3	5:C:2117:HOH:O	2.05	0.55
2:B:415:ASN:HB2	5:B:2143:HOH:O	2.07	0.55
3:A:1298:JYM:N9	5:A:2041:HOH:O	2.24	0.55
1:C:265:GLN:HA	1:C:268:HIS:CD2	2.42	0.54
1:A:15:TYR:N	1:A:15:TYR:HD1	2.06	0.54
1:C:40:GLU:HB3	1:C:41:THR:OG1	2.08	0.54
1:A:181:SER:HB3	5:A:2111:HOH:O	2.08	0.53
1:C:12:GLU:HG2	1:C:17:VAL:HG22	1.89	0.53
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:THR:C	5:B:2074:HOH:O	2.47	0.52
1:A:295:HIS:CD2	1:A:296:LEU:HG	2.44	0.52
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.90	0.52
2:D:395:HIS:HE1	2:D:427:PRO:O	1.93	0.52
2:D:176:PRO:HB2	2:D:179:HIS:NE2	2.26	0.51
2:D:407:GLN:O	2:D:411:GLU:HG2	2.11	0.50
2:B:296:HIS:CD2	2:B:300:LYS:HE3	2.46	0.50
1:A:9:LYS:NZ	1:A:12:GLU:HG2	2.27	0.50
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.42	0.49
1:A:71:HIS:HD2	1:A:76:LEU:HD13	1.75	0.49
1:C:51:GLU:O	1:C:55:LEU:HB2	2.12	0.49
1:A:9:LYS:HZ1	1:A:11:GLY:C	2.16	0.48
1:A:51:GLU:O	1:A:55:LEU:HB2	2.13	0.48
1:A:249:SER:HA	1:A:260:ARG:HD3	1.95	0.48
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.95	0.48
1:A:197:VAL:HG11	1:A:252:VAL:HG12	1.96	0.47
1:C:91:MET:HE1	1:C:130:PRO:HG2	1.97	0.47
5:C:2048:HOH:O	2:D:296:HIS:HD2	1.97	0.47
1:C:40:GLU:CA	1:C:41:THR:CB	2.91	0.47
1:C:154:VAL:O	2:D:316:THR:HG22	2.12	0.47
1:A:72:THR:O	2:B:296:HIS:NE2	2.47	0.47
2:D:176:PRO:HD2	2:D:179:HIS:CE1	2.49	0.47
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.97	0.46
1:C:34:LYS:HG3	1:C:77:TYR:CE2	2.50	0.46
1:C:34:LYS:HD3	1:C:75:LYS:HD2	1.98	0.46
1:C:290:THR:HG22	5:C:2061:HOH:O	2.15	0.46
1:A:265:GLN:HA	1:A:268:HIS:CD2	2.51	0.46
1:A:9:LYS:NZ	1:A:17:VAL:HG13	2.30	0.46
1:C:1:MET:N	5:C:2003:HOH:O	2.25	0.46
1:C:105:LYS:HE2	1:C:285:PHE:O	2.15	0.46
1:A:210:ASP:OD1	5:A:2122:HOH:O	2.21	0.45
1:C:40:GLU:HA	1:C:41:THR:OG1	2.14	0.45
2:D:196:LYS:HG3	2:D:244:SER:HB3	1.96	0.45
1:A:119:HIS:CD2	1:A:182:THR:HB	2.52	0.45
1:C:227:TRP:HB3	1:C:230:VAL:HG22	1.99	0.45
1:C:41:THR:HA	2:D:292:LEU:HD21	1.99	0.44
1:A:69:VAL:CG1	1:A:76:LEU:HD11	2.47	0.44
1:C:49:ILE:HG23	2:D:306:LEU:HD12	2.00	0.44
2:B:206:ILE:HG22	2:B:210:MET:HE1	2.00	0.44
1:C:20:LYS:HG3	1:C:82:PHE:CE1	2.52	0.44
1:A:84[B]:HIS:CE1	1:A:297:ARG:NH2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.99	0.44
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.53	0.44
2:B:177:ASP:N	5:B:2001:HOH:O	2.50	0.44
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.54	0.43
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.00	0.43
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.99	0.43
1:A:295:HIS:CE1	5:A:2189:HOH:O	2.71	0.43
1:A:295:HIS:H	1:A:296:LEU:HB2	1.82	0.43
1:C:75:LYS:HE3	1:C:77:TYR:OH	2.18	0.43
1:A:227:TRP:HB3	1:A:230:VAL:HG22	2.01	0.43
2:B:282:THR:O	2:B:285:THR:N	2.53	0.42
2:D:262:LEU:HD11	2:D:266:LYS:HE3	2.01	0.42
2:B:210:MET:HE1	2:B:250:ARG:HB3	2.01	0.42
1:C:74:ASN:ND2	1:C:74:ASN:H	2.17	0.42
1:C:40:GLU:CB	1:C:41:THR:OG1	2.67	0.42
2:D:177:ASP:C	2:D:179:HIS:H	2.22	0.42
2:D:177:ASP:O	2:D:179:HIS:N	2.53	0.42
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.02	0.42
1:A:297:ARG:HB2	5:A:2046:HOH:O	2.20	0.42
2:B:263:LEU:HD21	2:B:295:GLU:HG3	2.02	0.42
1:C:88:LYS:CB	1:C:131[B]:GLN:HG3	2.50	0.42
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.55	0.42
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.86	0.41
1:C:88:LYS:HB2	1:C:131[B]:GLN:HG3	2.01	0.41
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.35	0.41
2:D:373:PRO:HD2	2:D:376:LEU:HD12	2.02	0.41
1:C:224:GLU:OE2	1:C:231:THR:OG1	2.34	0.41
2:D:347:TYR:OH	2:D:394:LEU:HA	2.21	0.41
2:D:388:LYS:O	2:D:392:MET:HG2	2.21	0.41
2:B:347:TYR:OH	2:B:394:LEU:HA	2.21	0.41
1:A:295:HIS:CB	1:A:296:LEU:HB2	2.50	0.41
1:A:268:HIS:HB3	5:A:2169:HOH:O	2.21	0.41
2:D:176:PRO:CD	2:D:179:HIS:CE1	3.04	0.41
1:C:161:HIS:HD2	5:C:2095:HOH:O	2.03	0.40
1:C:227:TRP:O	1:C:230:VAL:HG22	2.22	0.40
1:C:227:TRP:O	1:C:230:VAL:CG2	2.70	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:C:217:ARG:NH1	5:A:2189:HOH:O[2_555]	1.96	0.24

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%)	287 (98%)	5 (2%)	2 (1%)	22	22
1	C	296/302 (98%)	289 (98%)	5 (2%)	2 (1%)	22	22
2	B	250/258 (97%)	248 (99%)	2 (1%)	0	100	100
2	D	251/258 (97%)	245 (98%)	5 (2%)	1 (0%)	34	37
All	All	1091/1120 (97%)	1069 (98%)	17 (2%)	5 (0%)	29	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	LEU
1	A	164	VAL
1	C	164	VAL
2	D	178	TYR
1	C	145	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	262/264 (99%)	238 (91%)	24 (9%)	9	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	262/264 (99%)	246 (94%)	16 (6%)	18	21
2	B	228/232 (98%)	217 (95%)	11 (5%)	25	32
2	D	229/232 (99%)	216 (94%)	13 (6%)	20	24
All	All	981/992 (99%)	917 (94%)	64 (6%)	16	19

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	6	LYS
1	A	15	TYR
1	A	22	ARG
1	A	36	ARG
1	A	55	LEU
1	A	72	THR
1	A	74	ASN
1	A	83	LEU
1	A	97	THR
1	A	101	LEU
1	A	122	ARG
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	178	LYS
1	A	230	VAL
1	A	232	SER
1	A	247	ASP
1	A	248	PHE
1	A	255	LEU
1	A	290	THR
1	A	295	HIS
1	A	296	LEU
2	B	177	ASP
2	B	179	HIS
2	B	199	TYR
2	B	232	LEU
2	B	274	GLU
2	B	292	LEU
2	B	316	THR
2	B	348	LEU
2	B	384	LEU

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Mol	Chain	Res	Type
2	B	391	LEU
2	B	431	ASN
1	C	0	SER
1	C	41	THR
1	C	55	LEU
1	C	72	THR
1	C	74	ASN
1	C	76	LEU
1	C	88	LYS
1	C	101	LEU
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG
1	C	178	LYS
1	C	230	VAL
1	C	248	PHE
1	C	255	LEU
1	C	256	ASP
2	D	181	ASP
2	D	199	TYR
2	D	232	LEU
2	D	245	SER
2	D	274	GLU
2	D	292	LEU
2	D	296	HIS
2	D	316	THR
2	D	327	CYS
2	D	348	LEU
2	D	371	SER
2	D	384	LEU
2	D	403	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	74	ASN
1	A	119	HIS
1	A	268	HIS
1	A	295	HIS
2	B	254	GLN
2	B	395	HIS

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Mol	Chain	Res	Type
2	B	425	ASN
2	B	431	ASN
1	C	59	ASN
1	C	71	HIS
1	C	113	GLN
1	C	119	HIS
1	C	268	HIS
2	D	296	HIS
2	D	317	GLN
2	D	323	GLN
2	D	395	HIS
2	D	396	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	C	160	1	8,10,11	0.74	0	10,14,16	1.03	0
1	TPO	A	160	1	8,10,11	0.63	0	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	C	160	1	-	0/9/11/13	-
1	TPO	A	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	JYM	C	1295	-	20,24,24	2.46	6 (30%)	24,35,35	1.97	9 (37%)
3	JYM	A	1298	-	20,24,24	1.64	4 (20%)	24,35,35	1.83	7 (29%)
4	DTT	B	1433	-	7,7,7	0.49	0	4,8,8	2.26	1 (25%)
4	DTT	D	1433	-	7,7,7	1.34	1 (14%)	4,8,8	3.11	1 (25%)

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	JYM	C	1295	-	-	3/11/19/19	0/3/3/3
3	JYM	A	1298	-	-	4/11/19/19	0/3/3/3
4	DTT	B	1433	-	-	3/8/8/8	-
4	DTT	D	1433	-	1/1/2/2	5/8/8/8	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1295	JYM	FAT-CAS	-6.61	1.08	1.32
3	C	1295	JYM	FAU-CAS	-5.55	1.12	1.32
3	A	1298	JYM	FAU-CAS	-4.61	1.16	1.32
3	C	1295	JYM	FAV-CAS	-3.83	1.18	1.32
3	C	1295	JYM	C5-C4	-3.22	1.32	1.40
3	C	1295	JYM	O6-C6	3.12	1.37	1.35
3	A	1298	JYM	FAT-CAS	-3.03	1.21	1.32
4	D	1433	DTT	C4-S4	2.58	1.87	1.81
3	A	1298	JYM	FAV-CAS	-2.37	1.24	1.32
3	A	1298	JYM	CAQ-CAR	2.21	1.59	1.53
3	C	1295	JYM	C6-N1	2.01	1.35	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1433	DTT	O2-C2-C3	5.83	121.69	109.72
4	B	1433	DTT	O2-C2-C3	4.48	118.92	109.72
3	A	1298	JYM	CAO-CAN-CAM	-4.22	104.17	112.15
3	C	1295	JYM	N3-C2-N1	-4.04	121.84	127.22
3	A	1298	JYM	O6-C6-N1	3.92	123.51	120.12
3	C	1295	JYM	O6-C6-N1	3.61	123.24	120.12
3	A	1298	JYM	N3-C2-N1	-3.48	122.58	127.22
3	C	1295	JYM	FAT-CAS-C8	-2.94	104.75	112.67
3	A	1298	JYM	CAL-O6-C6	-2.75	114.87	117.50
3	C	1295	JYM	C2-N3-C4	2.70	118.44	115.36
3	C	1295	JYM	FAU-CAS-C8	-2.68	105.46	112.67
3	C	1295	JYM	CAN-CAM-CAL	-2.51	104.99	111.28
3	A	1298	JYM	C2-N3-C4	2.25	117.92	115.36
3	C	1295	JYM	CAL-O6-C6	-2.21	115.39	117.50
3	A	1298	JYM	N2-C2-N3	2.19	121.36	117.79
3	C	1295	JYM	FAV-CAS-FAU	2.11	113.46	105.72
3	A	1298	JYM	CAQ-CAR-CAM	-2.08	108.22	112.15
3	C	1295	JYM	FAU-CAS-FAT	2.03	113.17	105.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	1433	DTT	C2

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1298	JYM	O6-CAL-CAM-CAR
4	B	1433	DTT	S1-C1-C2-C3
4	B	1433	DTT	O2-C2-C3-O3
4	B	1433	DTT	O2-C2-C3-C4
4	D	1433	DTT	S1-C1-C2-O2
4	D	1433	DTT	S1-C1-C2-C3
4	D	1433	DTT	O2-C2-C3-O3
4	D	1433	DTT	O2-C2-C3-C4
3	A	1298	JYM	O6-CAL-CAM-CAN
3	A	1298	JYM	CAM-CAL-O6-C6
3	C	1295	JYM	O6-CAL-CAM-CAN
3	C	1295	JYM	O6-CAL-CAM-CAR
3	A	1298	JYM	C5-C6-O6-CAL
3	C	1295	JYM	CAM-CAL-O6-C6
4	D	1433	DTT	C2-C3-C4-S4

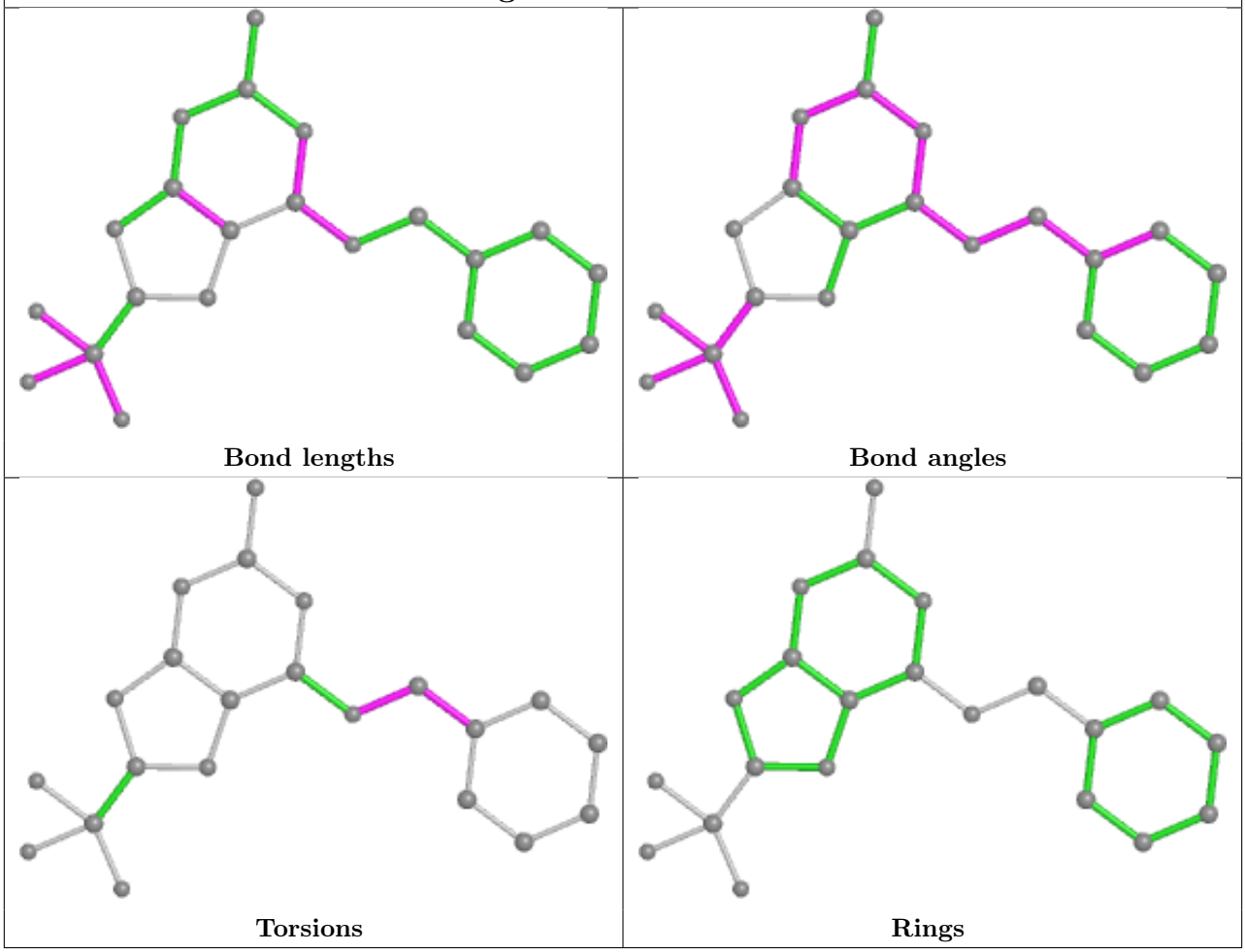
There are no ring outliers.

1 monomer is involved in 7 short contacts:

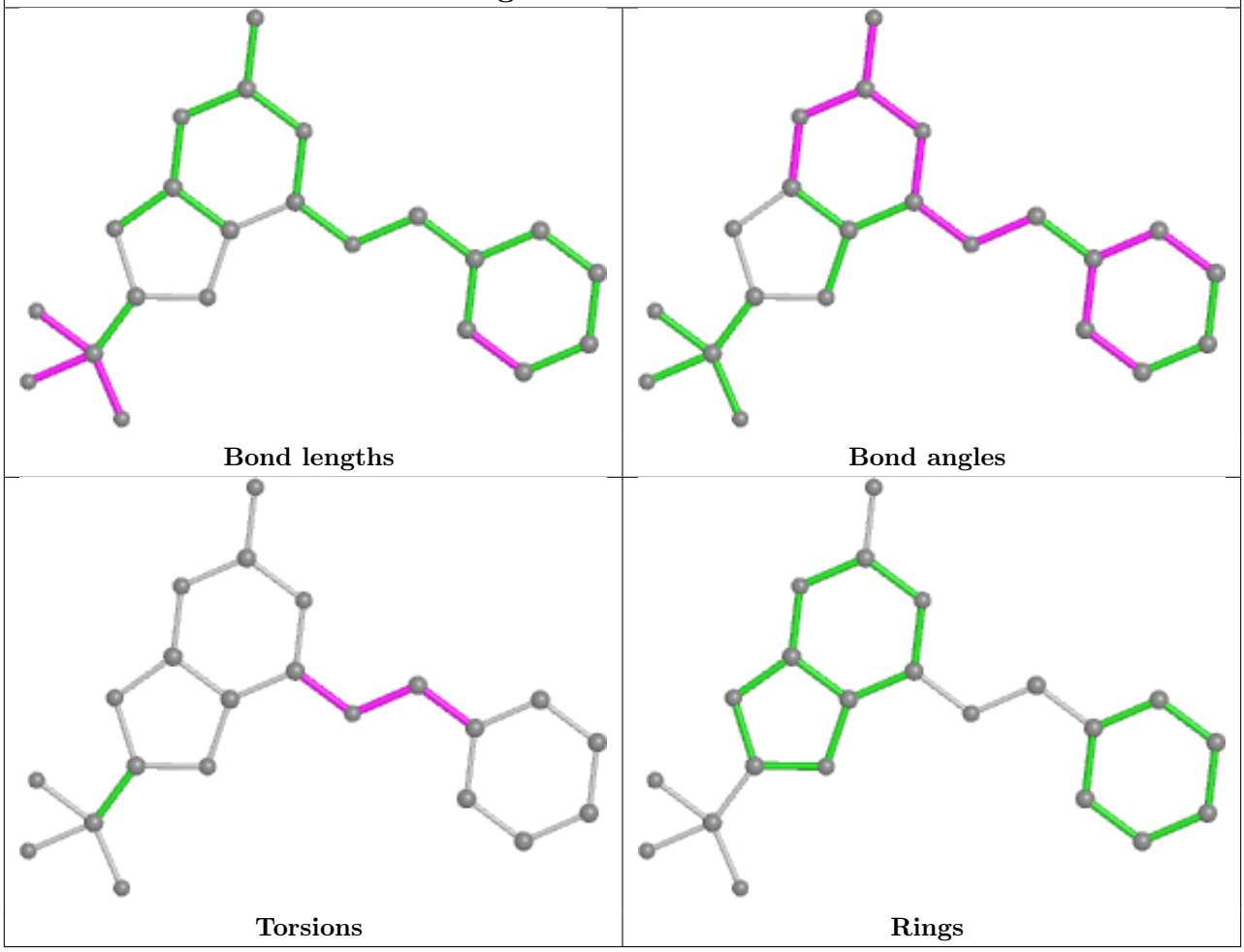
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	JYM	7	0

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 then 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.

Ligand JYM C 1295



Ligand JYM A 1298



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	296/302 (98%)	-0.09	13 (4%)	34	32	19, 28, 53, 65	1 (0%)
1	C	296/302 (98%)	-0.14	6 (2%)	65	63	28, 39, 54, 61	1 (0%)
2	B	254/258 (98%)	-0.36	1 (0%)	92	91	21, 30, 43, 55	1 (0%)
2	D	255/258 (98%)	0.05	13 (5%)	28	26	25, 42, 71, 89	1 (0%)
All	All	1101/1120 (98%)	-0.14	33 (2%)	50	48	19, 35, 59, 89	4 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ALA	5.6
1	A	14	THR	5.2
2	D	431	ASN	4.3
2	D	324	PRO	4.3
1	C	0	SER	4.2
2	D	176	PRO	4.1
1	A	15	TYR	3.8
1	A	96	LEU	3.6
1	C	287	GLN	3.5
1	A	84[A]	HIS	3.1
1	C	-2	PRO	2.8
1	A	295	HIS	2.8
1	A	13	GLY	2.7
2	D	323	GLN	2.7
2	D	415	ASN	2.5
2	D	418	TYR	2.5
1	A	16	GLY	2.5
1	C	232	SER	2.4
2	D	325	ALA	2.4
2	D	424	LEU	2.4
2	D	326	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	97	THR	2.3
1	A	71	HIS	2.2
2	D	327	CYS	2.2
2	D	419	HIS	2.2
1	A	94	SER	2.2
2	B	431	ASN	2.1
1	A	73	GLU	2.1
1	C	282	ALA	2.1
2	D	420	GLY	2.1
1	A	296	LEU	2.0
2	D	177	ASP	2.0
1	C	256	ASP	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	A	160	11/12	0.98	0.11	23,25,26,27	0
1	TPO	C	160	11/12	0.98	0.12	30,33,35,36	0

6.3 Carbohydrates (i)

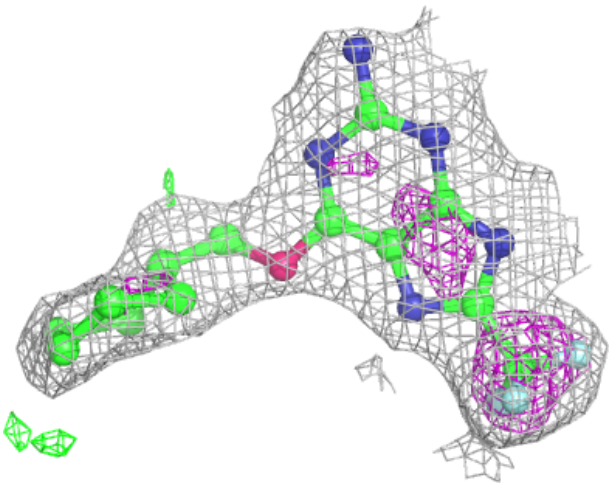
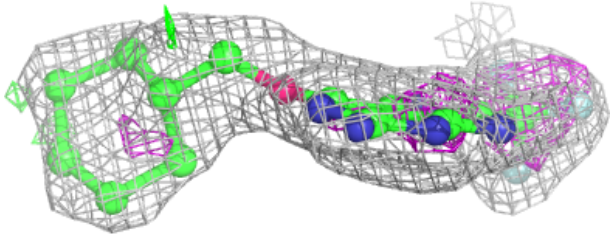
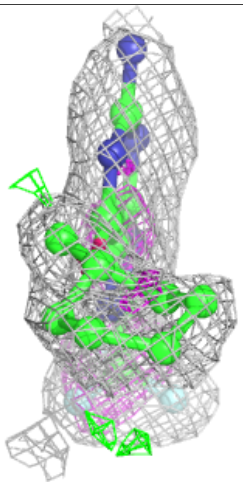
There are no monosaccharides in this entry.

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.

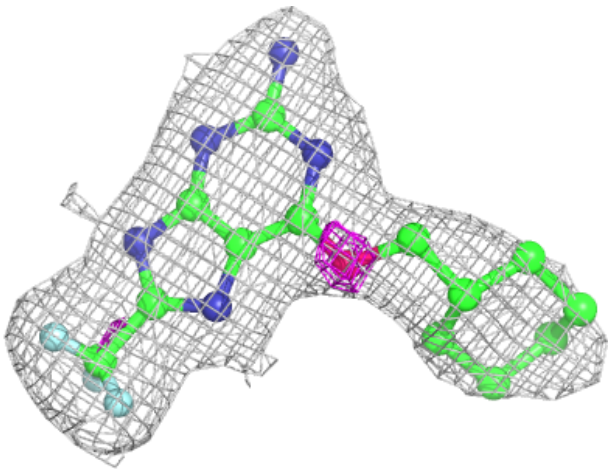
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	JYM	A	1298	22/22	0.90	0.19	40,43,47,50	0
4	DTT	D	1433	8/8	0.94	0.14	40,41,42,43	0
3	JYM	C	1295	22/22	0.95	0.12	36,38,43,45	0
4	DTT	B	1433	8/8	0.96	0.19	40,41,42,45	0

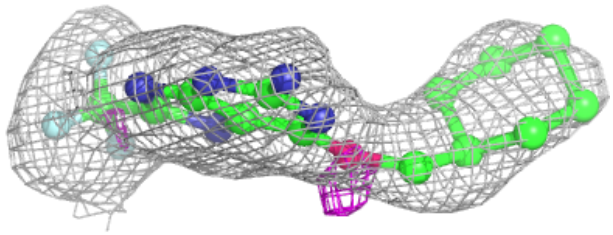
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

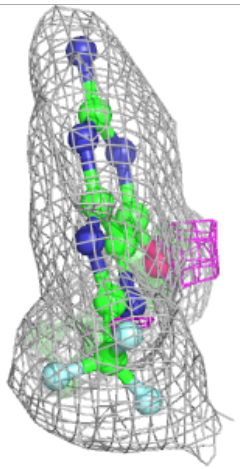
Electron density around JYM A 1298: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around JYM C 1295:

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.