



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 05:37 pm BST

PDB ID : 4CFV / pdb_00004cfv
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.; Echaliér,
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 : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

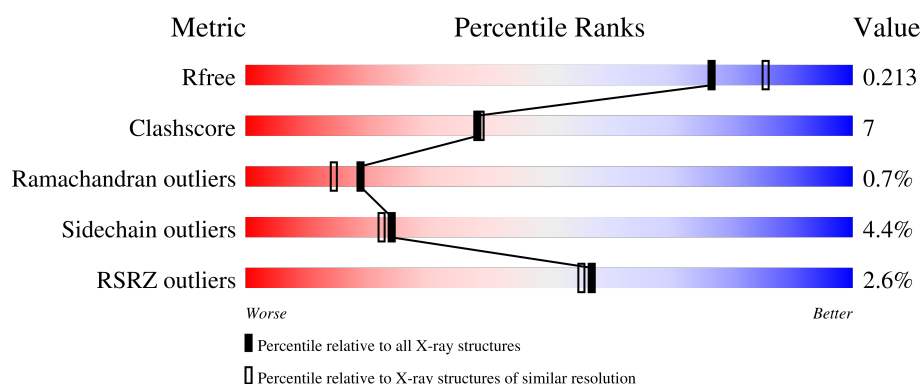
1 Overall quality at a glance

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	303	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>
1	C	303	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>• 13%</div> </div> </div>
2	B	262	<div> <div>0%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div> </div>
2	D	262	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	P	S	0	9	0
			2480	1608	421	441	1	9			
1	C	265	Total	C	N	O	P	S	0	5	0
			2169	1408	369	384	1	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-4	GLY	-	expression tag	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	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
2	B	262	Total	C	N	O	S		0	5	0
			2143	1388	349	396	10				
2	D	262	Total	C	N	O	S		0	3	0
			2130	1378	346	396	10				

There are 16 discrepancies between the modelled and reference sequences:

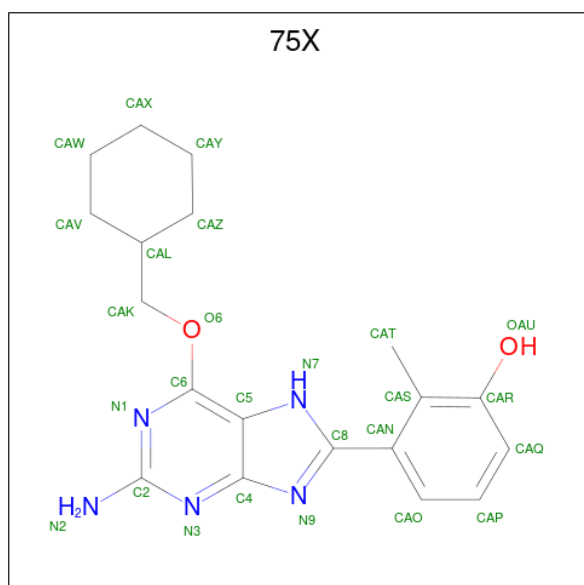
Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP P20248
B	311	ILE	VAL	conflict	UNP P20248

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Chain	Residue	Modelled	Actual	Comment	Reference
B	357	ALA	GLY	conflict	UNP P20248
B	377	VAL	ILE	conflict	UNP P20248
B	378	GLN	ARG	conflict	UNP P20248
B	386	THR	SER	conflict	UNP P20248
B	392	LEU	MET	conflict	UNP P20248
B	400	ARG	LYS	conflict	UNP P20248
D	171	GLY	-	expression tag	UNP P20248
D	311	ILE	VAL	conflict	UNP P20248
D	357	ALA	GLY	conflict	UNP P20248
D	377	VAL	ILE	conflict	UNP P20248
D	378	GLN	ARG	conflict	UNP P20248
D	386	THR	SER	conflict	UNP P20248
D	392	LEU	MET	conflict	UNP P20248
D	400	ARG	LYS	conflict	UNP P20248

- Molecule 3 is 3-[2-amino-6-(cyclohexylmethoxy)-7H-purin-8-yl]-2-methylphenol (CCD ID: 75X) (formula: C₁₉H₂₃N₅O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Mg 2	0	0
4	D	2	Total 2	Mg 2	0	0

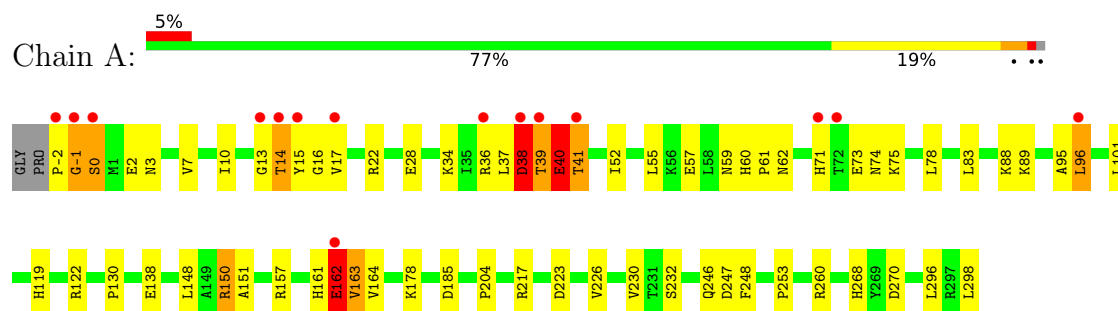
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	227	Total 227	O 227	0	0
5	B	170	Total 170	O 170	0	0
5	C	142	Total 142	O 142	0	0
5	D	123	Total 123	O 123	0	0

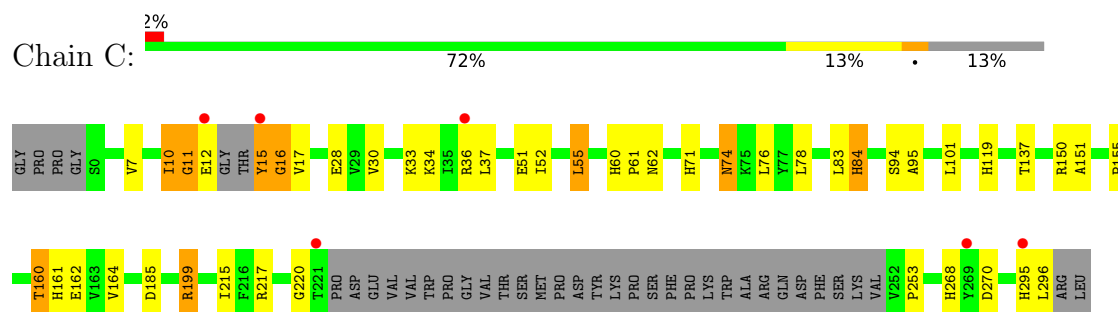
3 Residue-property plots

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.

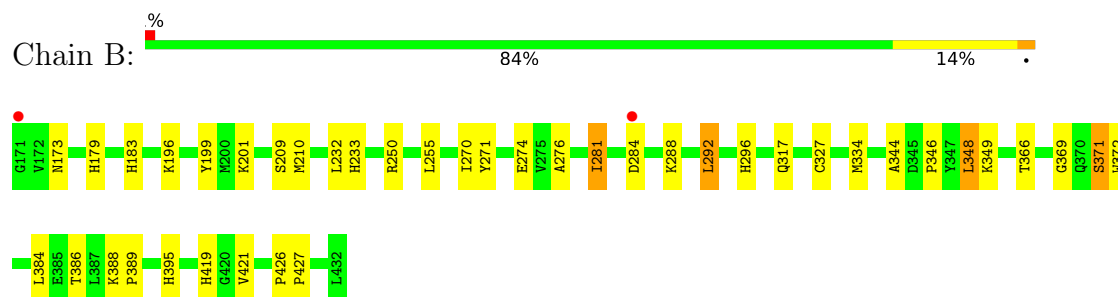
• Molecule 1: CYCLIN-DEPENDENT KINASE 2



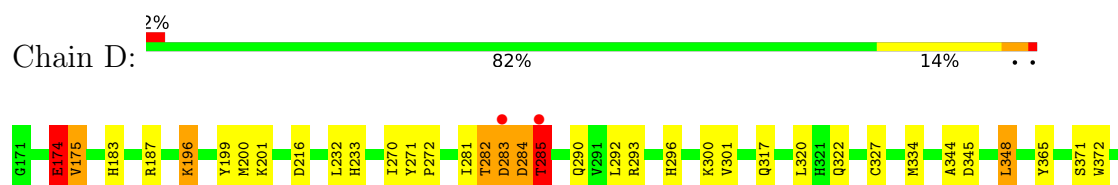
• Molecule 1: CYCLIN-DEPENDENT KINASE 2

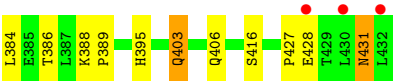


• Molecule 2: CYCLIN-A2



• Molecule 2: CYCLIN-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.07Å 133.91Å 147.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.00 19.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.87-2.00) 98.6 (19.87-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.178 , 0.205 0.185 , 0.213	Depositor DCC
R_{free} test set	4918 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.5	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	0.96	EDS
Total number of atoms	9640	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 75X, 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	1.39	9/2550 (0.4%)	1.28	15/3458 (0.4%)
1	C	1.30	6/2219 (0.3%)	1.20	6/3002 (0.2%)
2	B	1.33	9/2206 (0.4%)	1.22	8/2998 (0.3%)
2	D	1.30	13/2186 (0.6%)	1.32	13/2972 (0.4%)
All	All	1.33	37/9161 (0.4%)	1.26	42/12430 (0.3%)

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	4
1	C	0	1
2	D	0	2
All	All	0	7

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	426	PRO	CA-C	8.76	1.56	1.51
1	C	11	GLY	C-O	8.42	1.28	1.24
1	A	162	GLU	C-O	7.93	1.33	1.24
1	A	253	PRO	C-O	-7.62	1.16	1.24
1	A	-1	GLY	N-CA	7.57	1.53	1.45
2	D	174	GLU	C-O	-6.73	1.15	1.23
2	B	366	THR	C-O	-6.52	1.16	1.24
2	B	426	PRO	C-O	-6.26	1.19	1.25
2	D	290	GLN	C-O	-6.23	1.16	1.24
1	C	30	VAL	C-O	6.20	1.30	1.23
2	B	209	SER	C-O	6.03	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	369	GLY	C-O	-5.91	1.15	1.24
2	B	255	LEU	C-O	-5.91	1.17	1.24
2	D	301	VAL	C-O	-5.85	1.17	1.24
2	D	403	GLN	CA-C	-5.83	1.44	1.52
2	D	322	GLN	C-N	-5.81	1.29	1.33
1	A	204	PRO	CA-C	5.79	1.57	1.53
1	C	16	GLY	N-CA	5.73	1.54	1.45
2	B	276	ALA	N-CA	-5.71	1.39	1.46
2	D	285	THR	CA-C	5.68	1.60	1.52
2	B	292	LEU	CA-C	5.48	1.59	1.52
2	D	187	ARG	C-O	-5.48	1.17	1.24
2	D	345	ASP	N-CA	-5.47	1.39	1.45
2	D	175	VAL	N-CA	5.43	1.50	1.46
1	A	74	ASN	CA-C	-5.39	1.45	1.52
2	D	272	PRO	CA-C	5.39	1.54	1.51
1	A	10	ILE	CA-C	-5.34	1.45	1.52
2	B	270	ILE	C-O	-5.30	1.18	1.24
1	A	138	GLU	CA-C	5.25	1.60	1.52
1	A	217	ARG	C-O	-5.25	1.17	1.24
2	D	270	ILE	C-O	-5.22	1.18	1.24
1	A	163	VAL	N-CA	5.21	1.52	1.46
1	C	7	VAL	C-O	-5.18	1.18	1.23
1	C	151	ALA	C-O	-5.14	1.17	1.24
2	D	175	VAL	CA-C	5.11	1.58	1.52
2	D	416	SER	C-O	-5.09	1.17	1.24
1	C	215	ILE	C-O	5.04	1.29	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	175	VAL	N-CA-C	-17.80	90.53	108.15
2	D	174	GLU	N-CA-C	12.96	126.00	110.44
1	A	14	THR	N-CA-C	12.30	128.49	113.23
2	D	174	GLU	CA-C-N	10.93	135.27	123.25
2	D	174	GLU	C-N-CA	10.93	135.27	123.25
1	A	38	ASP	N-CA-C	-10.32	88.81	110.80
1	A	162	GLU	CA-C-N	8.77	134.96	122.77
1	A	162	GLU	C-N-CA	8.77	134.96	122.77
1	C	199	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	A	247	ASP	CA-C-O	7.80	128.22	120.88
2	B	334	MET	CG-SD-CE	-7.43	84.55	100.90
2	D	175	VAL	CB-CA-C	-7.38	104.07	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	GLN	N-CA-CB	7.26	121.35	110.53
2	B	271	TYR	CA-C-N	-7.13	114.45	119.66
2	B	271	TYR	C-N-CA	-7.13	114.45	119.66
1	C	10	ILE	CB-CA-C	-7.09	101.98	110.84
2	D	271	TYR	CA-C-N	-6.85	114.66	119.66
2	D	271	TYR	C-N-CA	-6.85	114.66	119.66
1	A	-1	GLY	CA-C-N	6.78	133.91	121.70
1	A	-1	GLY	C-N-CA	6.78	133.91	121.70
1	A	162	GLU	CB-CA-C	6.23	122.82	110.42
1	C	253	PRO	N-CA-C	6.22	118.29	110.70
2	D	334	MET	CG-SD-CE	-6.17	87.32	100.90
1	C	199	ARG	NE-CZ-NH1	6.15	127.65	121.50
2	D	174	GLU	CA-C-O	-6.06	114.08	121.89
1	C	74	ASN	N-CA-C	5.79	121.38	113.97
1	A	40	GLU	N-CA-C	-5.71	104.31	113.28
1	A	163	VAL	N-CA-C	-5.69	100.88	108.96
1	C	199	ARG	CD-NE-CZ	5.63	132.28	124.40
1	A	150	ARG	CA-CB-CG	5.47	125.05	114.10
2	B	281	ILE	N-CA-CB	5.43	122.45	111.05
2	B	371	SER	N-CA-C	5.41	118.40	109.85
2	B	199	TYR	N-CA-C	5.39	117.91	111.71
1	A	14	THR	CA-C-O	-5.33	113.03	119.27
1	A	247	ASP	CB-CA-C	5.30	116.32	109.80
2	D	386	THR	CB-CA-C	-5.29	101.86	110.85
2	D	270	ILE	N-CA-C	-5.25	105.42	110.72
1	A	7	VAL	N-CA-C	-5.24	107.06	111.56
1	A	157	ARG	CB-CA-C	-5.14	101.56	110.45
2	B	421	VAL	N-CA-C	5.11	117.44	111.05
2	D	174	GLU	O-C-N	-5.04	115.12	121.83
2	B	270	ILE	N-CA-C	-5.01	105.82	110.53

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	THR	Peptide
1	A	162	GLU	Peptide
1	A	37	LEU	Peptide
1	A	40	GLU	Peptide
1	C	220	GLY	Peptide
2	D	174	GLU	Peptide
2	D	282	THR	Peptide

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	2480	0	2527	50	0
1	C	2169	0	2222	35	0
2	B	2143	0	2162	23	0
2	D	2130	0	2142	25	0
3	A	26	0	23	1	0
3	C	26	0	22	1	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
5	A	227	0	0	16	2
5	B	170	0	0	9	0
5	C	142	0	0	7	1
5	D	123	0	0	5	0
All	All	9640	0	9098	123	2

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 7.

All (123) 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:122[B]:ARG:NH1	5:A:2092:HOH:O	1.95	0.98
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.83	0.96
1:A:95:ALA:O	1:A:96:LEU:HB2	1.67	0.95
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.00	0.93
1:A:22[B]:ARG:NH1	5:A:2016:HOH:O	2.05	0.90
1:A:161:HIS:O	1:A:162:GLU:C	2.15	0.89
2:D:282:THR:O	2:D:285:THR:OG1	1.91	0.87
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.90	0.86
1:C:160:TPO:CG2	1:C:162[B]:GLU:HG3	2.06	0.86
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.56	0.86
1:A:260:ARG:HD3	5:A:2191:HOH:O	1.77	0.83
1:C:160:TPO:HG23	1:C:162[B]:GLU:HG3	1.60	0.83
1:C:60:HIS:HD2	1:C:62:ASN:H	1.29	0.81
2:B:210:MET:HE1	2:B:250:ARG:CB	2.10	0.81
2:B:173[B]:ASN:ND2	5:B:2016:HOH:O	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:HD2	1:A:62:ASN:H	1.30	0.78
1:A:161:HIS:HD2	5:A:2045:HOH:O	1.68	0.77
1:A:57:GLU:O	5:A:2051:HOH:O	2.04	0.75
1:C:84[A]:HIS:NE2	1:C:296:LEU:HD13	2.02	0.75
1:A:60:HIS:CD2	1:A:62:ASN:H	2.07	0.72
1:C:15[A]:TYR:N	1:C:15[A]:TYR:CD1	2.57	0.72
1:A:59[A]:ASN:ND2	5:A:2055:HOH:O	2.22	0.71
1:C:84[A]:HIS:NE2	1:C:296:LEU:CD1	2.53	0.71
1:A:161:HIS:HE1	5:A:2130:HOH:O	1.71	0.71
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.56	0.71
1:C:60:HIS:CD2	1:C:62:ASN:H	2.09	0.70
1:A:246:GLN:O	5:A:2162:HOH:O	2.11	0.69
2:D:327:CYS:SG	5:D:2099:HOH:O	2.50	0.68
1:C:74:ASN:ND2	5:C:2025:HOH:O	2.24	0.67
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.74	0.65
2:B:210:MET:CE	2:B:250:ARG:HB2	2.25	0.64
1:A:-1:GLY:HA2	1:A:0:SER:HB2	1.81	0.62
1:C:95:ALA:HA	1:C:199:ARG:HD2	1.81	0.62
1:C:10:ILE:CG2	1:C:10:ILE:O	2.47	0.62
1:C:11:GLY:O	1:C:12:GLU:HG3	2.00	0.62
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.81	0.61
1:A:178:LYS:HE3	5:A:2125:HOH:O	2.01	0.61
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.83	0.61
2:B:296:HIS:HD2	5:B:2100:HOH:O	1.85	0.59
1:C:10:ILE:O	1:C:10:ILE:HG22	2.03	0.59
2:B:183:HIS:HD2	5:B:2029:HOH:O	1.85	0.59
2:D:372:TRP:HB3	2:D:384:LEU:HD11	1.85	0.59
1:A:28:GLU:OE2	5:A:2023:HOH:O	2.17	0.58
1:C:119:HIS:HD2	5:C:2076:HOH:O	1.84	0.58
1:A:38:ASP:O	1:A:38:ASP:CG	2.47	0.56
1:C:161:HIS:HD2	5:C:2039:HOH:O	1.87	0.56
2:B:233:HIS:HD2	5:B:2109:HOH:O	1.88	0.55
2:B:395:HIS:HE1	2:B:427:PRO:O	1.90	0.55
2:B:179[A]:HIS:CE1	5:B:2022:HOH:O	2.59	0.54
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.71	0.54
1:C:15[B]:TYR:CE2	1:C:36:ARG:HB2	2.43	0.53
2:D:200:MET:HB2	5:D:2030:HOH:O	2.07	0.53
1:A:39:THR:O	1:A:40:GLU:HB3	2.07	0.53
1:A:41:THR:HB	2:B:288:LYS:NZ	2.23	0.53
1:A:119:HIS:HD2	5:A:2090:HOH:O	1.91	0.53
1:A:268:HIS:HD2	1:A:270:ASP:H	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2035:HOH:O	2:B:274:GLU:HG2	2.09	0.53
1:A:3:ASN:OD1	2:D:293:ARG:NH1	2.41	0.53
2:B:386:THR:HB	5:B:2146:HOH:O	2.09	0.53
1:A:122[B]:ARG:CZ	1:A:151:ALA:HB1	2.39	0.52
1:A:13:GLY:HA3	5:A:2009:HOH:O	2.10	0.51
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.94	0.51
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.93	0.51
1:A:161:HIS:HB3	5:A:2129:HOH:O	2.11	0.51
1:A:15[B]:TYR:CB	1:A:16:GLY:HA2	2.41	0.50
1:A:38:ASP:O	1:A:40:GLU:N	2.44	0.50
1:A:60:HIS:HE1	5:A:2014:HOH:O	1.94	0.50
2:D:395:HIS:HE1	2:D:427:PRO:O	1.94	0.49
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.95	0.49
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.47	0.49
1:A:248:PHE:O	5:A:2190:HOH:O	2.19	0.48
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.95	0.48
1:A:15[B]:TYR:CB	1:A:16:GLY:CA	2.91	0.48
1:A:39:THR:O	1:A:40:GLU:CB	2.61	0.48
1:C:94:SER:O	1:C:199:ARG:HD3	2.15	0.47
1:C:217:ARG:HD2	5:C:2129:HOH:O	2.14	0.47
1:C:268:HIS:HD2	1:C:270:ASP:H	1.63	0.47
1:A:2[B]:GLU:HG3	2:D:293:ARG:HH22	1.78	0.47
1:A:223:ASP:H	1:A:226:VAL:HG12	1.79	0.47
1:C:11:GLY:C	1:C:12:GLU:HG3	2.39	0.47
1:C:137:THR:HA	1:C:296:LEU:HD12	1.97	0.47
1:C:155:PRO:HG3	2:D:320:LEU:HD21	1.96	0.47
1:C:12:GLU:HG2	1:C:16:GLY:O	2.14	0.47
3:C:1297:75X:HAX	5:C:2085:HOH:O	2.15	0.47
1:C:295:HIS:H	1:C:295:HIS:CD2	2.32	0.46
2:B:386:THR:CB	5:B:2146:HOH:O	2.64	0.46
1:A:83:LEU:O	3:A:1299:75X:N9	2.48	0.46
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.51	0.46
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.84	0.46
2:D:371:SER:O	2:D:372:TRP:C	2.58	0.45
1:A:38:ASP:O	1:A:39:THR:C	2.60	0.45
1:A:15[B]:TYR:HB3	1:A:16:GLY:CA	2.47	0.44
2:B:233:HIS:HE1	5:B:2110:HOH:O	1.99	0.44
1:A:161:HIS:O	1:A:162:GLU:O	2.36	0.44
1:C:84[A]:HIS:NE2	1:C:296:LEU:HD11	2.30	0.44
5:C:2054:HOH:O	2:D:296:HIS:HD2	1.99	0.44
1:C:84[A]:HIS:CE1	1:C:296:LEU:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ASP:HB2	5:B:2094:HOH:O	2.17	0.43
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.00	0.43
2:D:216:ASP:HB2	2:D:406:GLN:HG2	1.99	0.43
1:A:41:THR:HB	2:B:288:LYS:HZ3	1.82	0.43
1:A:95:ALA:O	1:A:96:LEU:CB	2.43	0.43
1:C:51:GLU:O	1:C:55:LEU:HB2	2.19	0.43
2:D:283[A]:ASP:O	2:D:284:ASP:HB2	2.18	0.42
2:D:196:LYS:HG2	2:D:199:TYR:HB3	2.01	0.42
2:D:365:TYR:OH	2:D:431:ASN:OD1	2.35	0.42
1:C:15[B]:TYR:HA	1:C:16:GLY:HA2	1.79	0.42
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.54	0.42
1:C:28:GLU:OE2	5:C:2015:HOH:O	2.21	0.42
2:D:201:LYS:NZ	5:D:2035:HOH:O	2.21	0.42
1:A:88:LYS:HB2	1:A:130:PRO:HB2	2.01	0.42
1:A:-1:GLY:CA	1:A:0:SER:HB2	2.49	0.42
1:A:15[B]:TYR:CE2	1:A:36:ARG:HD2	2.55	0.42
2:D:233:HIS:HE1	5:D:2091:HOH:O	2.01	0.42
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.02	0.41
2:B:371:SER:O	2:B:372:TRP:C	2.62	0.41
2:B:346:PRO:O	2:B:349:LYS:HG2	2.21	0.41
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.92	0.41
2:B:327:CYS:HB3	2:B:419:HIS:CE1	2.55	0.41
2:D:233:HIS:HD2	5:D:2090:HOH:O	2.04	0.40
1:A:-2:PRO:O	2:D:300:LYS:HD3	2.22	0.40
1:A:38:ASP:C	1:A:40:GLU:H	2.29	0.40
1:A:230:VAL:C	1:A:232:SER:H	2.29	0.40

All (2) 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)
5:A:2160:HOH:O	5:A:2214:HOH:O[4_555]	2.02	0.18
5:A:2224:HOH:O	5:C:2126:HOH:O[3_454]	2.12	0.08

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	307/303 (101%)	293 (95%)	10 (3%)	4 (1%)	10	5
1	C	262/303 (86%)	255 (97%)	6 (2%)	1 (0%)	30	27
2	B	265/262 (101%)	262 (99%)	3 (1%)	0	100	100
2	D	263/262 (100%)	256 (97%)	3 (1%)	4 (2%)	8	4
All	All	1097/1130 (97%)	1066 (97%)	22 (2%)	9 (1%)	19	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	96	LEU
1	A	164	VAL
1	C	164	VAL
2	D	284	ASP
1	A	162	GLU
2	D	431	ASN
2	D	283[A]	ASP
2	D	283[B]	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	273/265 (103%)	259 (95%)	14 (5%)	20	17
1	C	237/265 (89%)	224 (94%)	13 (6%)	18	15
2	B	239/235 (102%)	232 (97%)	7 (3%)	37	39
2	D	237/235 (101%)	227 (96%)	10 (4%)	25	24
All	All	986/1000 (99%)	942 (96%)	44 (4%)	24	21

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	34	LYS
1	A	38	ASP
1	A	39	THR
1	A	41	THR
1	A	73	GLU
1	A	75	LYS
1	A	89	LYS
1	A	101	LEU
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	296	LEU
1	A	298	LEU
2	B	196	LYS
2	B	201	LYS
2	B	232	LEU
2	B	281	ILE
2	B	292	LEU
2	B	348	LEU
2	B	384	LEU
1	C	15[A]	TYR
1	C	15[B]	TYR
1	C	17	VAL
1	C	33	LYS
1	C	34	LYS
1	C	37	LEU
1	C	55	LEU
1	C	76	LEU
1	C	83	LEU
1	C	84[A]	HIS
1	C	84[B]	HIS
1	C	101	LEU
1	C	150	ARG
2	D	174	GLU
2	D	175	VAL
2	D	196	LYS
2	D	232	LEU
2	D	281	ILE
2	D	285	THR
2	D	292	LEU
2	D	348	LEU
2	D	403	GLN

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Mol	Chain	Res	Type
2	D	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	119	HIS
1	A	161	HIS
1	A	246	GLN
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	313	GLN
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
1	C	60	HIS
1	C	71	HIS
1	C	119	HIS
1	C	161	HIS
1	C	265	GLN
1	C	268	HIS
1	C	295	HIS
2	D	173	ASN
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	313	GLN
2	D	317	GLN
2	D	395	HIS
2	D	396	GLN
2	D	425	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	C	160	1	8,10,11	1.14	1 (12%)	10,14,16	1.29	2 (20%)
1	TPO	A	160	1	8,10,11	1.00	0	10,14,16	1.18	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	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	2.03	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-2.11	119.25	124.78
1	C	160	TPO	O3P-P-O2P	2.03	115.39	107.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	75X	C	1297	-	27,29,29	2.17	9 (33%)	31,41,41	2.81	16 (51%)
3	75X	A	1299	-	27,29,29	1.96	5 (18%)	31,41,41	2.27	8 (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	75X	C	1297	-	-	4/9/17/17	0/4/4/4
3	75X	A	1299	-	-	5/9/17/17	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1299	75X	CAN-C8	-4.78	1.37	1.48
3	C	1297	75X	CAN-C8	-4.75	1.37	1.48
3	A	1299	75X	CAT-CAS	-4.63	1.42	1.51
3	C	1297	75X	CAR-CAS	4.08	1.44	1.40
3	C	1297	75X	O6-C6	3.98	1.38	1.35
3	C	1297	75X	CAT-CAS	-3.85	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1297	75X	CAY-CAZ	3.37	1.62	1.53
3	A	1299	75X	CAO-CAN	3.23	1.45	1.40
3	A	1299	75X	C6-N1	3.11	1.37	1.31
3	C	1297	75X	CAO-CAN	2.97	1.44	1.40
3	A	1299	75X	CAY-CAZ	2.91	1.60	1.53
3	C	1297	75X	C2-N2	-2.72	1.28	1.33
3	C	1297	75X	C6-N1	2.56	1.36	1.31
3	C	1297	75X	C8-N7	2.11	1.38	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1299	75X	CAN-C8-N7	5.80	131.07	123.67
3	C	1297	75X	O6-CAK-CAL	-5.37	94.19	108.21
3	C	1297	75X	CAN-C8-N7	5.31	130.45	123.67
3	A	1299	75X	CAY-CAZ-CAL	-4.89	102.90	112.15
3	C	1297	75X	CAQ-CAR-CAS	4.86	126.62	121.61
3	A	1299	75X	O6-CAK-CAL	-4.75	95.81	108.21
3	C	1297	75X	CAW-CAV-CAL	-4.72	103.24	112.15
3	C	1297	75X	N2-C2-N3	4.65	125.37	117.79
3	C	1297	75X	CAY-CAZ-CAL	-4.57	103.51	112.15
3	A	1299	75X	N3-C2-N1	-4.39	121.37	127.22
3	C	1297	75X	N3-C2-N1	-3.79	122.17	127.22
3	A	1299	75X	N2-C2-N3	3.30	123.17	117.79
3	C	1297	75X	N2-C2-N1	-3.13	112.39	117.25
3	A	1299	75X	C8-N9-C4	3.12	111.94	103.76
3	C	1297	75X	CAT-CAS-CAR	2.99	124.36	120.84
3	C	1297	75X	CAP-CAQ-CAR	-2.95	116.32	120.05
3	C	1297	75X	CAP-CAO-CAN	2.91	125.24	120.33
3	A	1299	75X	CAW-CAV-CAL	-2.90	106.66	112.15
3	A	1299	75X	O6-C6-N1	2.89	122.62	120.12
3	C	1297	75X	CAO-CAN-CAS	-2.78	116.96	119.92
3	C	1297	75X	O6-C6-N1	-2.67	117.82	120.12
3	C	1297	75X	CAN-C8-N9	-2.47	120.53	123.67
3	C	1297	75X	C8-N9-C4	2.30	109.77	103.76
3	C	1297	75X	C2-N3-C4	2.12	117.78	115.36

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1299	75X	N7-C8-CAN-CAO

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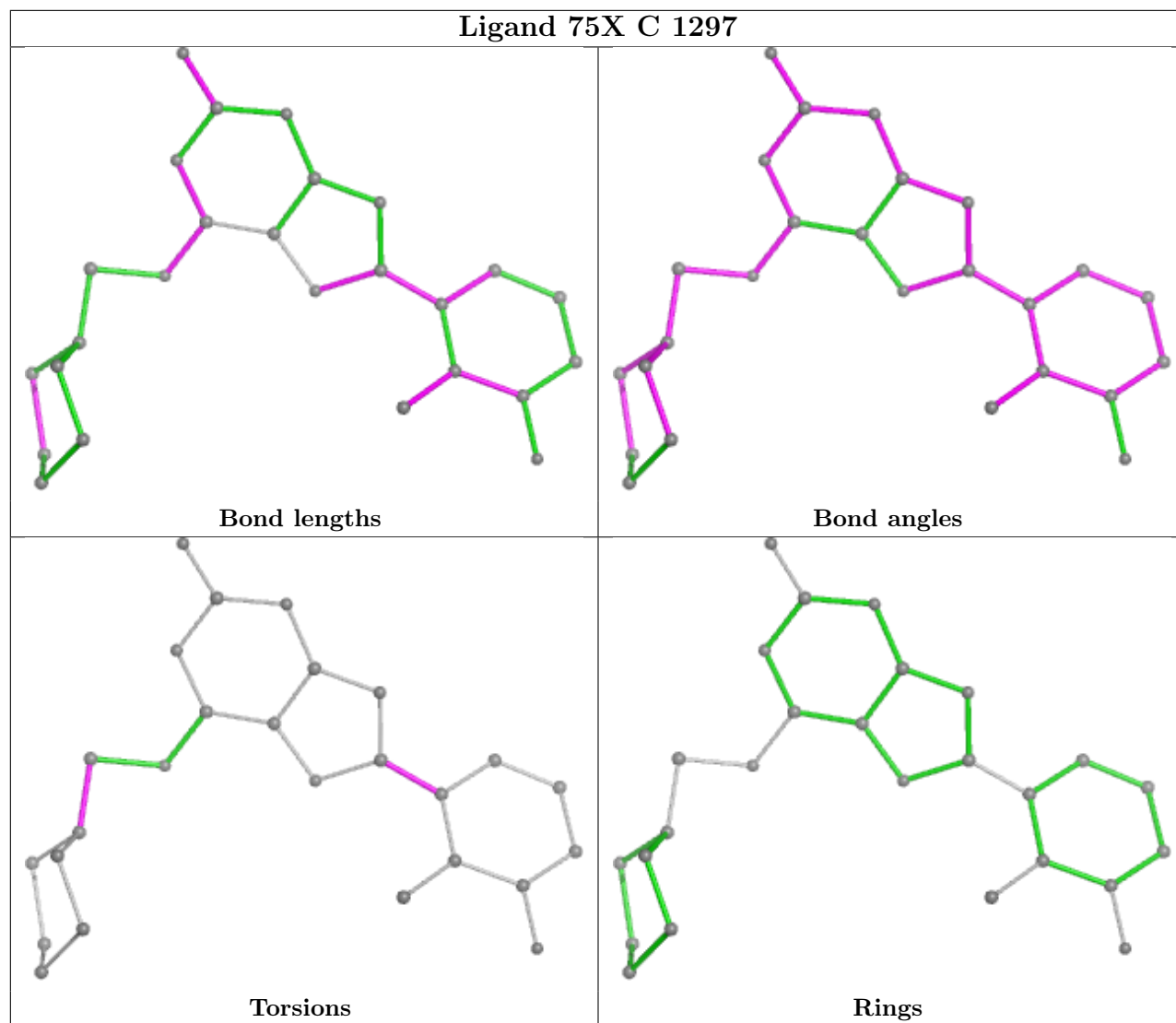
Mol	Chain	Res	Type	Atoms
3	A	1299	75X	O6-CAK-CAL-CAV
3	A	1299	75X	O6-CAK-CAL-CAZ
3	C	1297	75X	N7-C8-CAN-CAO
3	C	1297	75X	O6-CAK-CAL-CAV
3	C	1297	75X	O6-CAK-CAL-CAZ
3	A	1299	75X	CAL-CAK-O6-C6
3	A	1299	75X	N9-C8-CAN-CAO
3	C	1297	75X	N9-C8-CAN-CAO

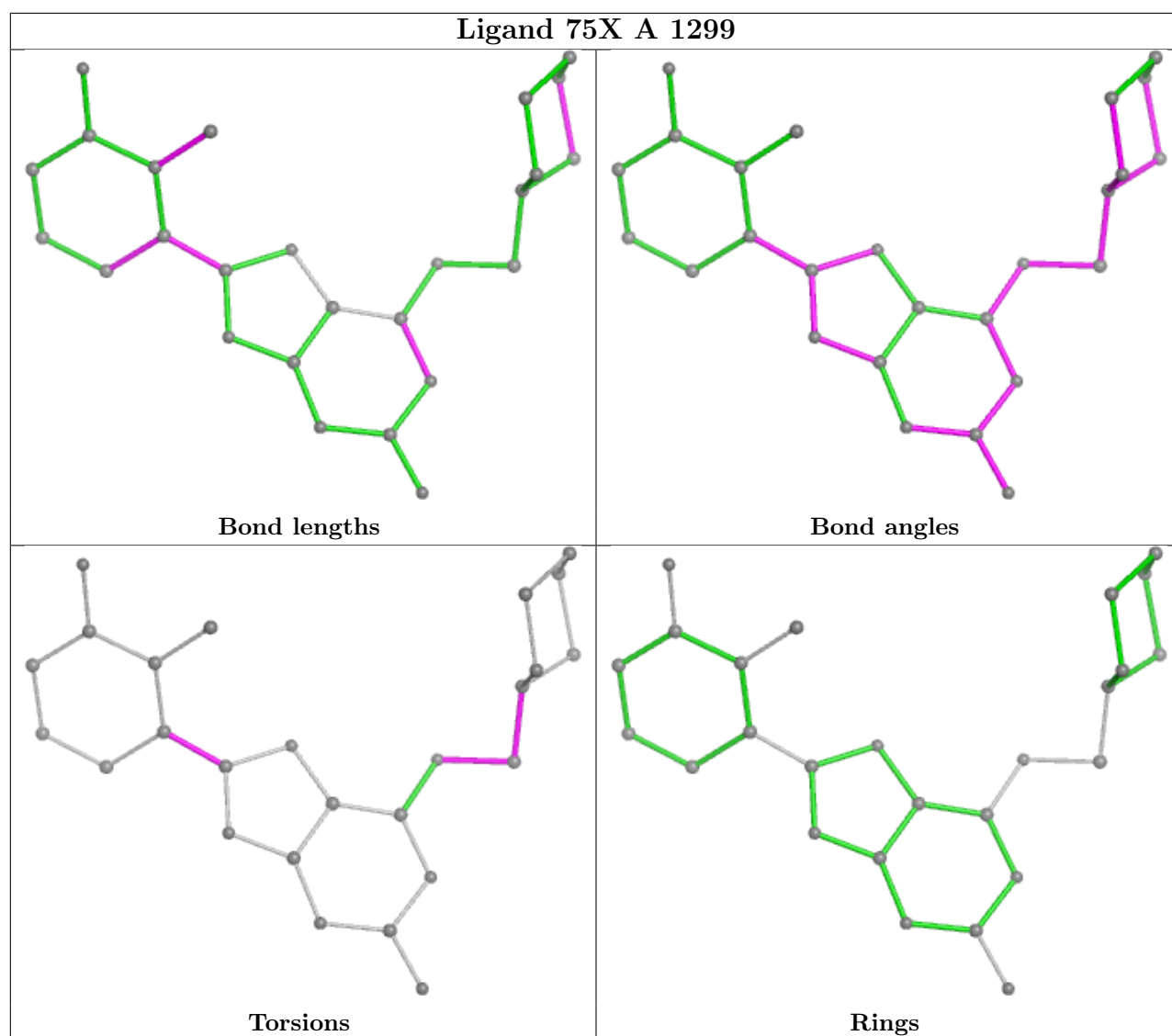
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	75X	1	0
3	A	1299	75X	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	300/303 (99%)	-0.36	15 (5%) 35 33	9, 24, 51, 76	9 (3%)
1	C	264/303 (87%)	-0.17	6 (2%) 61 59	18, 32, 49, 62	5 (1%)
2	B	262/262 (100%)	-0.50	2 (0%) 82 82	13, 27, 41, 56	5 (1%)
2	D	262/262 (100%)	-0.15	5 (1%) 66 65	18, 35, 68, 94	3 (1%)
All	All	1088/1130 (96%)	-0.30	28 (2%) 57 55	9, 29, 56, 94	22 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15[A]	TYR	5.3
1	A	41	THR	4.7
1	A	39	THR	4.5
1	A	71	HIS	4.5
1	A	96	LEU	4.0
1	A	14	THR	3.8
1	A	162	GLU	3.3
1	A	15[A]	TYR	3.3
1	C	295	HIS	3.3
2	D	283[A]	ASP	3.2
2	D	432	LEU	3.2
1	A	13	GLY	2.9
2	B	284	ASP	2.9
1	A	38	ASP	2.9
2	B	171	GLY	2.8
1	C	36	ARG	2.7
1	A	17	VAL	2.7
1	A	0	SER	2.6
1	C	269	TYR	2.6
2	D	430	LEU	2.5
1	C	221	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	-2	PRO	2.3
1	A	36	ARG	2.3
2	D	285	THR	2.3
1	A	-1	GLY	2.3
1	C	12	GLU	2.2
2	D	428	GLU	2.2
1	A	72	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.97	0.06	24,27,29,30	0
1	TPO	A	160	11/12	0.98	0.05	20,22,23,23	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.

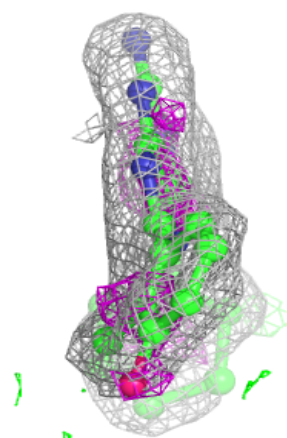
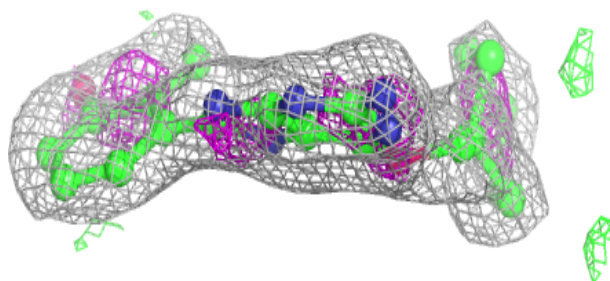
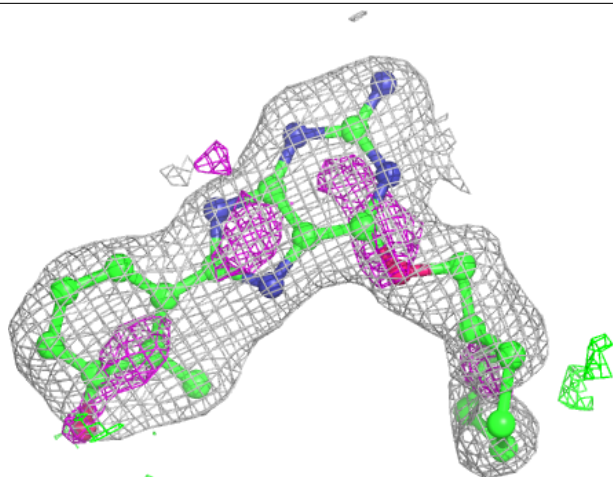
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	75X	C	1297	26/26	0.81	0.13	28,40,44,46	0
3	75X	A	1299	26/26	0.86	0.11	28,36,43,44	0
4	MG	D	1433	1/1	0.94	0.09	34,34,34,34	0
4	MG	B	1434	1/1	0.97	0.06	32,32,32,32	0
4	MG	B	1433	1/1	0.97	0.15	32,32,32,32	0
4	MG	D	1434	1/1	0.97	0.09	32,32,32,32	0

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.

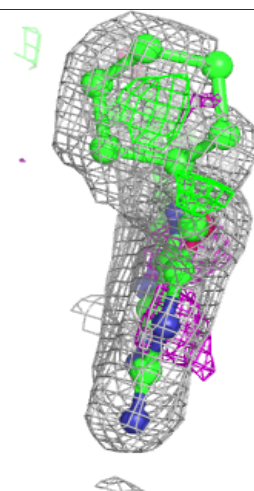
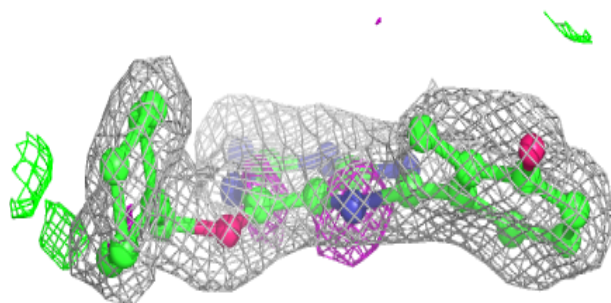
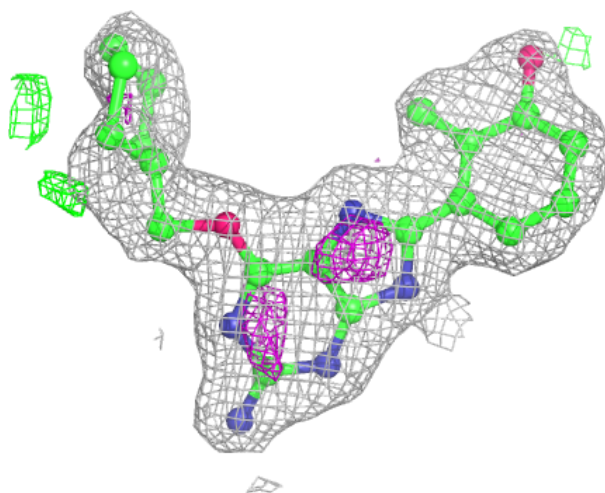
Electron density around 75X C 1297:

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



Electron density around 75X A 1299:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.