



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:16 AM UTC

PDB ID : 2IW6 / pdb_00002iw6
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2-CYCLIN A COM-
PLEXED WITH A BISANILINOPYRIMIDINE INHIBITOR
Authors : Pratt, D.J.; Bentley, J.; Jewsbury, P.; Boyle, F.T.; Endicott, J.A.; Noble,
M.E.M.
Deposited on : 2006-06-26
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

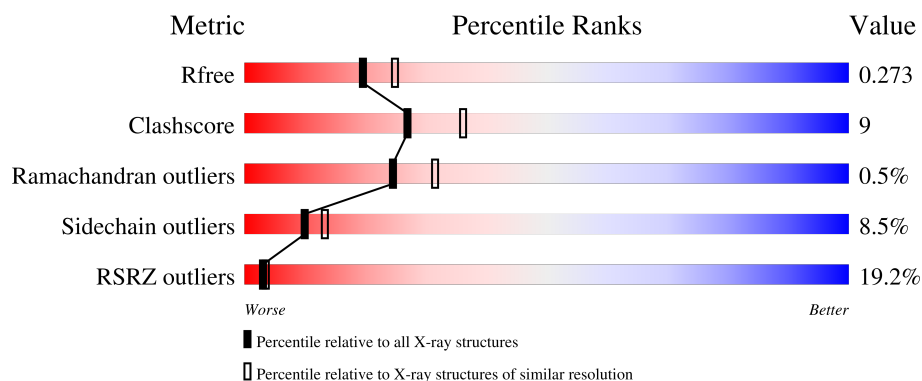
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	12% 67% 26% ...
1	C	302	26% 71% 22% 5% .
2	B	260	9% 80% 17% ..
2	D	260	28% 72% 20% 6% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9062 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	293	Total	C	N	O	P	S	0	0	0
			2354	1529	399	417	1	8			
1	C	296	Total	C	N	O	P	S	0	0	0
			2378	1542	402	425	1	8			

There are 10 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	0	0
			2076	1345	338	382	11			
2	D	255	Total	C	N	O	S	0	0	0
			2061	1336	336	378	11			

There are 2 discrepancies between the modelled and reference sequences:

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

- # QQ2
-
- The chemical structure is a complex organic molecule with the following features:
- Top Group:** A quaternary ammonium cation with a central nitrogen atom (N30) bonded to three methyl groups (C29, C31, C32) and a propyl chain (C28-C27-C26).
 - Chiral Center:** The C26 carbon is a chiral center, bonded to the propyl chain, a hydroxyl group (O33), and a benzyl ether group (C25-O-C23).
 - Phenyl Ether:** A benzene ring (C21-C24) is connected to the ether oxygen (O25). It has an amine group (NH2, N19) at the para position (C23) and a pyridine ring at the other para position (C21).
 - Pyridine Ring:** A six-membered aromatic ring with one nitrogen atom (N6) and a cyano group (C4-N5) at the 3-position.
 - Substituted Benzene:** A benzene ring (C8-C13) is connected to the pyridine ring at its 4-position (C3). It has a chlorine atom (Cl1) at the 2-position (C10) and a cyano group (C16-N18) at the 1-position (C9).
- Atom labels include: C29, C31, C32, N30, C28, C27, C26, O33, C25, O25, C24, C23, C22, C21, N19, N6, C4, C3, C2, C1, N5, C13, C12, C11, C10, C9, Cl1, C16, C17, N18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 33	C 24	Cl 1	N 6	O 2	0	0
3	C	1	Total 33	C 24	Cl 1	N 6	O 2	0	0

- SGM
-
- The diagram shows the chemical structure of (S)-butane-2,3-diol-1-thiol, labeled SGM. The molecule consists of a four-carbon chain. The first carbon (C1) is bonded to a thiol group (-SH), with the sulfur atom labeled S1. The second carbon (C2) is bonded to a hydroxyl group (-OH) with a dashed bond, indicating it is on the opposite side of the plane from the thiol group. The third carbon (C3) is bonded to a hydroxyl group (-OH) with a wedged bond, indicating it is on the same side of the plane as the thiol group. The fourth carbon is bonded to a hydrogen atom (not explicitly shown). The carbons are labeled C1, C2(R), and C3 in green. The hydroxyl groups are labeled OH and the thiol group is labeled SH in red. The sulfur atom is labeled S1 in green.

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		

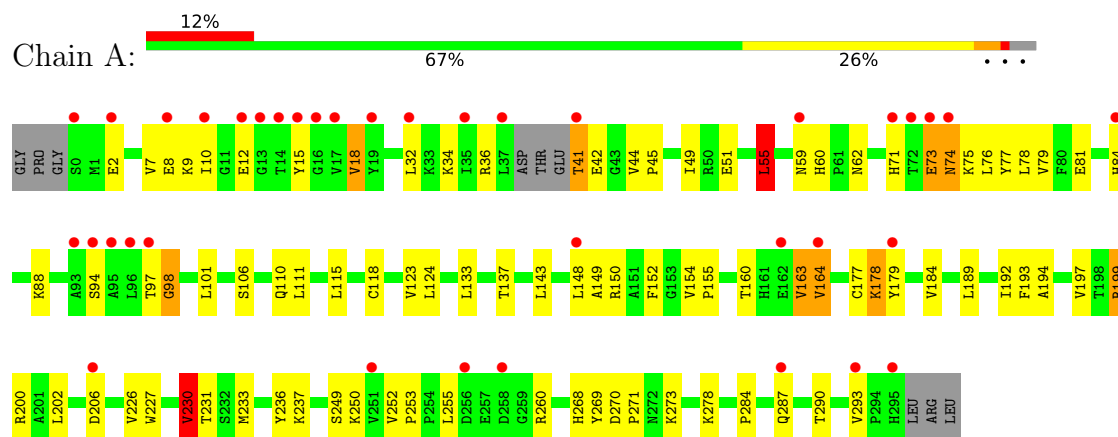
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		
6	B	49	Total	O	0	0
			49	49		
6	C	9	Total	O	0	0
			9	9		
6	D	8	Total	O	0	0
			8	8		

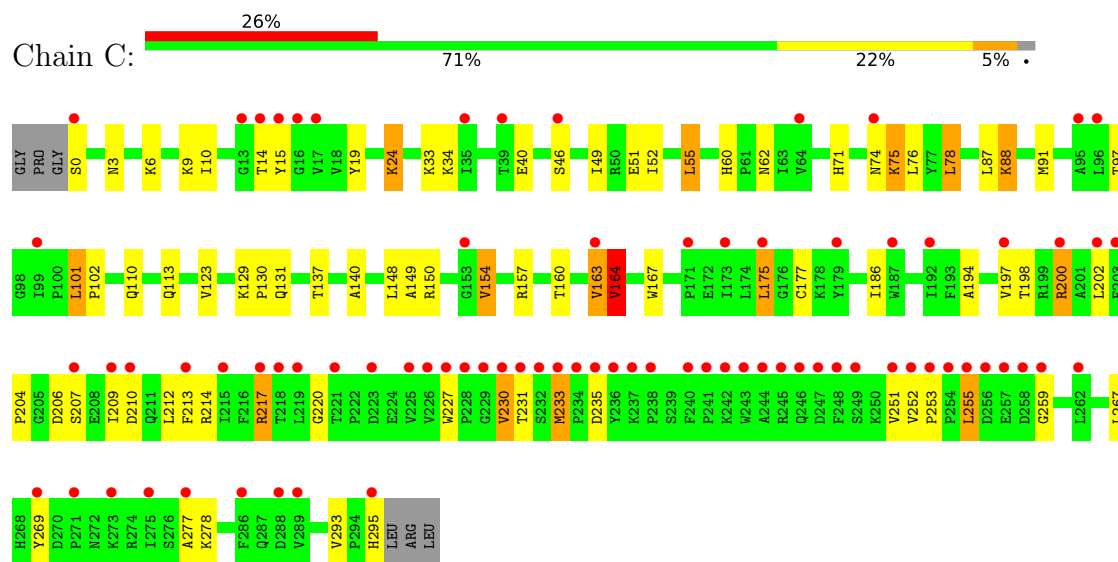
3 Residue-property plots [i](#)

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

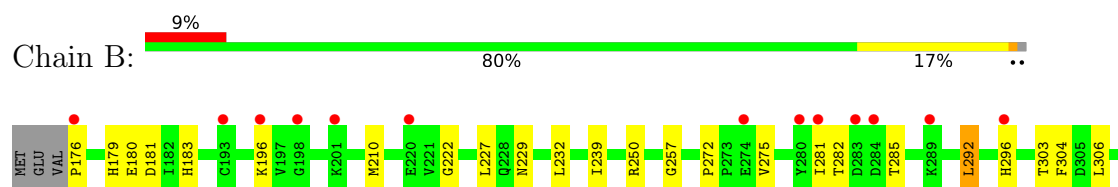
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

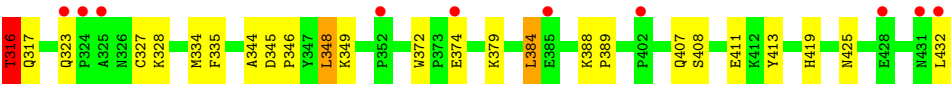


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

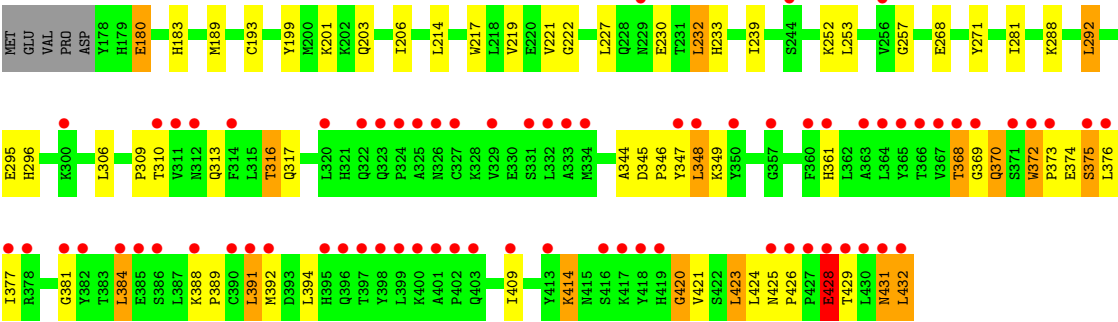


• Molecule 2: CYCLIN-A2





● Molecule 2: CYCLIN-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.78Å 134.56Å 148.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 99.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.1 (100.00-2.30) 92.6 (99.64-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.287 0.218 , 0.273	Depositor DCC
R_{free} test set	3125 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.0	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	0.90	EDS
Total number of atoms	9062	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 2.97% 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, SGM, MG, QQ2

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	1.06	2/2403 (0.1%)	1.21	13/3260 (0.4%)
1	C	0.81	1/2428 (0.0%)	1.06	5/3296 (0.2%)
2	B	0.99	1/2126 (0.0%)	1.19	4/2886 (0.1%)
2	D	1.55	31/2110 (1.5%)	1.22	16/2864 (0.6%)
All	All	1.12	35/9067 (0.4%)	1.17	38/12306 (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
2	D	0	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	423	LEU	C-O	21.55	1.49	1.24
2	D	429	THR	C-N	17.66	1.56	1.33
2	D	420	GLY	C-N	15.15	1.54	1.33
2	D	421	VAL	C-N	15.06	1.53	1.33
2	D	375	SER	CB-OG	12.63	1.67	1.42
2	D	370	GLN	CD-OE1	12.22	1.46	1.23
2	D	423	LEU	C-N	12.20	1.50	1.33
2	D	421	VAL	C-O	11.79	1.38	1.24
2	D	381	GLY	C-N	11.57	1.49	1.33
2	D	369	GLY	C-N	10.15	1.48	1.33
2	D	425	ASN	CG-ND2	10.06	1.54	1.33
2	D	425	ASN	CG-OD1	9.70	1.42	1.23
2	D	428	GLU	C-O	-9.48	1.12	1.24
2	D	428	GLU	CA-CB	8.75	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	429	THR	CA-CB	7.87	1.65	1.53
2	D	368	THR	CB-OG1	7.71	1.56	1.43
2	D	420	GLY	C-O	7.39	1.34	1.24
2	D	370	GLN	C-O	7.30	1.33	1.23
2	D	431	ASN	C-O	7.20	1.33	1.23
2	D	414	LYS	CE-NZ	7.13	1.70	1.49
2	D	381	GLY	C-O	7.08	1.34	1.23
2	D	424	LEU	CG-CD2	6.35	1.73	1.52
2	D	429	THR	CB-OG1	6.25	1.53	1.43
1	A	118	CYS	C-O	-6.10	1.17	1.24
2	D	426	PRO	N-CD	6.02	1.56	1.47
1	A	123	VAL	CA-CB	5.78	1.61	1.54
2	D	429	THR	CA-C	5.75	1.60	1.52
2	D	374	GLU	CD-OE2	5.67	1.36	1.25
2	D	428	GLU	C-N	5.62	1.41	1.33
2	D	425	ASN	C-O	5.58	1.31	1.24
2	B	272	PRO	CA-C	5.49	1.55	1.52
2	D	425	ASN	C-N	5.45	1.39	1.33
2	D	377	ILE	C-N	5.38	1.41	1.33
2	D	424	LEU	N-CA	5.31	1.53	1.46
1	C	123	VAL	CA-CB	5.19	1.60	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	423	LEU	O-C-N	9.21	131.89	122.12
1	A	230	VAL	CB-CA-C	-8.71	100.63	112.04
2	D	425	ASN	OD1-CG-ND2	7.56	130.16	122.60
1	A	253	PRO	N-CA-C	7.18	119.46	110.70
1	A	84	HIS	N-CA-C	6.93	118.83	111.28
1	A	270	ASP	CA-C-N	6.64	126.89	119.32
1	A	270	ASP	C-N-CA	6.64	126.89	119.32
1	C	253	PRO	N-CA-C	6.40	118.51	110.70
1	A	55	LEU	N-CA-C	5.90	118.49	111.71
2	D	429	THR	CA-C-N	-5.83	113.51	122.60
2	D	429	THR	C-N-CA	-5.83	113.51	122.60
1	A	110	GLN	N-CA-C	5.79	117.59	111.28
1	C	149	ALA	N-CA-C	5.78	118.21	110.35
2	D	420	GLY	O-C-N	5.76	129.70	122.39
2	B	272	PRO	CA-C-N	-5.74	113.86	119.78
2	B	272	PRO	C-N-CA	-5.74	113.86	119.78
2	D	421	VAL	O-C-N	5.72	129.73	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	316	THR	N-CA-CB	-5.66	101.80	110.12
2	D	381	GLY	O-C-N	5.62	129.20	122.34
2	B	408	SER	N-CA-C	5.61	118.33	111.82
2	D	372	TRP	CA-C-N	5.56	125.50	119.78
2	D	372	TRP	C-N-CA	5.56	125.50	119.78
1	C	233	MET	CA-C-N	5.53	125.62	119.32
1	C	233	MET	C-N-CA	5.53	125.62	119.32
2	D	271	TYR	CA-C-N	-5.52	114.69	120.38
2	D	271	TYR	C-N-CA	-5.52	114.69	120.38
2	D	369	GLY	CA-C-O	5.39	124.78	118.96
1	A	193	PHE	N-CA-C	-5.34	105.36	111.07
1	C	52	ILE	N-CA-C	5.33	115.54	110.53
2	D	429	THR	N-CA-C	-5.32	101.62	109.18
2	D	295	GLU	CA-C-N	5.19	127.19	120.44
2	D	295	GLU	C-N-CA	5.19	127.19	120.44
1	A	230	VAL	N-CA-CB	5.18	116.95	110.47
1	A	115	LEU	N-CA-C	5.03	116.57	111.14
1	A	98	GLY	CA-C-N	-5.03	118.42	123.04
1	A	98	GLY	C-N-CA	-5.03	118.42	123.04
1	A	18	VAL	N-CA-C	5.01	115.06	107.80
2	D	423	LEU	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	428	GLU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2354	0	2395	56	0
1	C	2378	0	2413	43	0
2	B	2076	0	2098	36	0
2	D	2061	0	2086	40	0
3	A	33	0	27	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	33	0	27	5	0
4	B	6	0	7	0	0
4	D	6	0	7	1	0
5	B	1	0	0	0	0
6	A	48	0	0	3	0
6	B	49	0	0	1	0
6	C	9	0	0	1	0
6	D	8	0	0	1	0
All	All	9062	0	9060	165	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:414:LYS:CE	2:D:414:LYS:NZ	1.70	1.53
2:D:375:SER:OG	2:D:375:SER:CB	1.67	1.40
2:D:193:CYS:SG	4:D:1433:SGM:S1	2.30	1.29
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.17	1.13
1:C:177:CYS:HB2	1:C:233:MET:HE3	1.12	1.11
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.20	1.07
1:A:284:PRO:O	1:A:287:GLN:HG2	1.59	1.03
1:C:200:ARG:HH11	1:C:200:ARG:HG2	1.23	1.03
2:B:210:MET:HE1	2:B:250:ARG:CB	1.97	0.95
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.50	0.93
1:A:137:THR:O	1:A:293:VAL:HG13	1.68	0.92
2:B:229:ASN:HD22	2:B:334:MET:HE2	1.34	0.90
1:A:51:GLU:OE2	6:A:2006:HOH:O	1.88	0.90
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.09	0.87
2:B:210:MET:CE	2:B:250:ARG:HB2	2.06	0.83
1:A:2:GLU:HB3	6:A:2001:HOH:O	1.77	0.83
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.50	0.80
1:A:74:ASN:ND2	1:A:74:ASN:H	1.83	0.77
2:B:317:GLN:NE2	6:B:2032:HOH:O	2.09	0.77
1:C:154:VAL:O	2:D:316:THR:HG23	1.85	0.77
1:C:204:PRO:HD2	1:C:214:ARG:HD3	1.66	0.77
1:A:177:CYS:HB2	1:A:233:MET:CE	2.16	0.75
1:A:227:TRP:O	1:A:230:VAL:HG22	1.88	0.74
1:A:177:CYS:SG	1:A:179:TYR:O	2.44	0.73
1:A:154:VAL:O	2:B:316:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:O	2:B:316:THR:CG2	2.38	0.72
1:A:73:GLU:HG2	1:A:74:ASN:HD22	1.56	0.71
1:C:177:CYS:CB	1:C:233:MET:HE3	2.07	0.69
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.76	0.67
2:D:414:LYS:NZ	2:D:414:LYS:CD	2.58	0.67
2:D:203:GLN:O	6:D:2002:HOH:O	2.13	0.67
1:C:200:ARG:HG2	1:C:200:ARG:NH1	2.01	0.66
1:C:213:PHE:HB3	1:C:217:ARG:NH1	2.10	0.66
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.31	0.66
2:B:388:LYS:HG3	2:B:432:LEU:HD13	1.77	0.65
2:D:346:PRO:O	2:D:349:LYS:HG2	1.96	0.65
2:D:388:LYS:HE3	2:D:432:LEU:HB3	1.79	0.64
1:C:227:TRP:O	1:C:230:VAL:HG22	1.97	0.64
1:A:74:ASN:ND2	1:A:74:ASN:N	2.46	0.63
1:A:71:HIS:HD2	1:A:76:LEU:HD13	1.63	0.62
1:A:15:TYR:OH	1:A:51:GLU:OE1	2.12	0.62
1:C:198:THR:HG23	1:C:252:VAL:HG13	1.82	0.62
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.82	0.61
1:C:137:THR:O	1:C:293:VAL:HG13	2.00	0.61
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.83	0.60
1:A:71:HIS:CE1	2:B:296:HIS:CD2	2.90	0.60
1:C:87:LEU:O	1:C:91:MET:HG2	2.02	0.58
1:C:214:ARG:HA	1:C:217:ARG:HD2	1.86	0.58
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.85	0.58
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.85	0.57
2:B:275:VAL:HG11	2:B:292:LEU:CD1	2.34	0.57
2:D:375:SER:CB	2:D:375:SER:HG	2.10	0.57
1:A:269:TYR:O	1:A:271:PRO:HD3	2.04	0.57
2:D:347:TYR:OH	2:D:394:LEU:HA	2.04	0.57
1:A:278:LYS:NZ	2:B:181:ASP:OD2	2.30	0.56
1:A:74:ASN:HD22	1:A:74:ASN:N	2.04	0.55
1:A:41:THR:HG22	1:A:42:GLU:H	1.72	0.55
2:B:229:ASN:HD22	2:B:334:MET:CE	2.14	0.54
1:C:154:VAL:O	2:D:316:THR:CG2	2.55	0.54
1:A:111:LEU:HD22	1:A:133:LEU:HD22	1.90	0.54
1:C:34:LYS:HE3	1:C:75:LYS:HZ3	1.73	0.54
1:A:60:HIS:CD2	1:A:62:ASN:H	2.25	0.54
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.96	0.53
2:D:180:GLU:HA	2:D:180:GLU:OE1	2.08	0.53
2:D:368:THR:OG1	2:D:370:GLN:HG3	2.07	0.53
2:D:373:PRO:HD2	2:D:376:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:VAL:HG11	2:B:292:LEU:HD11	1.90	0.52
2:D:217:TRP:O	2:D:221:VAL:HG23	2.09	0.52
1:A:71:HIS:CE1	2:B:296:HIS:CG	2.97	0.52
2:B:407:GLN:O	2:B:411:GLU:HG2	2.10	0.51
1:C:60:HIS:CD2	1:C:62:ASN:H	2.28	0.51
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.93	0.51
1:C:207:SER:HB3	1:C:210:ASP:H	1.76	0.50
2:B:183:HIS:CD2	2:B:379:LYS:HE3	2.46	0.50
1:A:137:THR:O	1:A:293:VAL:CG1	2.51	0.50
1:A:231:THR:HA	1:A:236:TYR:CD1	2.47	0.50
3:C:1296:QQ2:H4	3:C:1296:QQ2:C21	2.41	0.50
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.47	0.49
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.94	0.49
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.95	0.49
1:C:110:GLN:HA	1:C:113:GLN:HE21	1.77	0.49
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.94	0.49
1:C:129:LYS:HE2	1:C:131:GLN:HB2	1.95	0.49
1:A:7:VAL:HG12	1:A:8:GLU:HG2	1.96	0.48
1:C:154:VAL:HG12	2:D:317:GLN:HG2	1.96	0.48
2:D:214:LEU:HD11	2:D:257:GLY:HA3	1.96	0.48
1:C:3:ASN:O	1:C:24:LYS:HG3	2.13	0.47
2:B:222:GLY:HA2	2:B:227:LEU:HD12	1.96	0.47
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.95	0.47
1:A:15:TYR:CD1	1:A:15:TYR:N	2.82	0.47
1:C:78:LEU:HD23	1:C:78:LEU:N	2.29	0.47
1:A:10:ILE:HD12	1:A:18:VAL:HG12	1.97	0.47
2:B:303:THR:O	2:B:304:PHE:HB2	2.13	0.47
1:C:200:ARG:HH11	1:C:200:ARG:CG	2.09	0.47
1:A:249:SER:HA	1:A:260:ARG:HD3	1.96	0.47
3:C:1296:QQ2:C21	3:C:1296:QQ2:C4	2.93	0.47
1:A:18:VAL:HG11	3:A:1296:QQ2:H9	1.96	0.46
2:B:372:TRP:HB3	2:B:384:LEU:HD13	1.98	0.46
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.30	0.46
3:C:1296:QQ2:C4	3:C:1296:QQ2:H21	2.46	0.46
2:D:420:GLY:O	2:D:423:LEU:N	2.44	0.46
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.50	0.45
3:C:1296:QQ2:H321	6:C:2009:HOH:O	2.16	0.45
2:B:388:LYS:HB3	2:B:389:PRO:CD	2.47	0.45
1:C:51:GLU:O	1:C:55:LEU:HB2	2.16	0.45
1:C:163:VAL:HG12	1:C:164:VAL:HG23	1.99	0.45
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:TYR:CE2	1:C:33:LYS:HE2	2.51	0.45
3:A:1296:QQ2:H4	3:A:1296:QQ2:C21	2.47	0.45
2:B:239:ILE:HD11	2:B:257:GLY:HA2	1.98	0.45
1:A:71:HIS:HE1	2:B:296:HIS:CD2	2.34	0.44
2:B:346:PRO:O	2:B:349:LYS:HG2	2.17	0.44
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.00	0.44
1:C:175:LEU:O	1:C:235:ASP:HB2	2.18	0.44
1:C:202:LEU:HD21	1:C:267:LEU:HD11	2.00	0.44
1:A:154:VAL:O	2:B:316:THR:HG23	2.18	0.43
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.48	0.43
1:C:49:ILE:HG23	2:D:306:LEU:HD12	2.00	0.43
3:A:1296:QQ2:H4	3:A:1296:QQ2:H21	2.00	0.43
1:C:251:VAL:HG12	1:C:252:VAL:HG23	2.00	0.43
2:D:239:ILE:HD11	2:D:257:GLY:HA2	2.01	0.43
1:C:10:ILE:HG22	3:C:1296:QQ2:H331	2.01	0.43
1:A:106:SER:HB2	1:A:290:THR:O	2.18	0.43
1:A:178:LYS:HB2	1:A:178:LYS:HE2	1.93	0.43
2:D:392:MET:HA	2:D:392:MET:HE2	2.00	0.43
1:A:124:LEU:O	1:A:149:ALA:HA	2.18	0.43
1:C:101:LEU:N	1:C:102:PRO:HD2	2.34	0.43
2:D:384:LEU:HD23	2:D:432:LEU:HD11	2.01	0.43
2:B:345:ASP:HA	2:B:346:PRO:HA	1.90	0.43
2:D:345:ASP:HA	2:D:346:PRO:HA	1.84	0.43
1:A:34:LYS:HG3	1:A:77:TYR:CE1	2.54	0.43
1:A:60:HIS:HE1	6:A:2004:HOH:O	2.01	0.42
2:B:327:CYS:HB3	2:B:419:HIS:CE1	2.54	0.42
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.84	0.42
2:D:252:LYS:HD2	2:D:252:LYS:HA	1.84	0.42
2:D:288:LYS:O	2:D:292:LEU:HB2	2.20	0.42
1:C:186:ILE:HD11	1:C:277:ALA:HB2	2.02	0.42
2:B:425:ASN:HD22	2:B:425:ASN:HA	1.67	0.42
1:C:220:GLY:O	1:C:269:TYR:OH	2.37	0.42
2:D:388:LYS:HB3	2:D:389:PRO:CD	2.50	0.42
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.55	0.41
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.50	0.41
3:A:1296:QQ2:H21	3:A:1296:QQ2:C4	2.50	0.41
2:D:206:ILE:HD13	2:D:253:LEU:HD13	2.03	0.41
2:D:233:HIS:HB3	2:D:310:THR:HB	2.01	0.41
1:A:81:GLU:O	1:A:81:GLU:HG3	2.19	0.41
1:C:110:GLN:OE1	1:C:140:ALA:HA	2.20	0.41
1:C:212:LEU:O	1:C:213:PHE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ARG:HE	1:C:217:ARG:HB3	1.62	0.41
1:A:250:LYS:HD3	1:A:250:LYS:HA	1.82	0.41
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.56	0.41
2:D:344:ALA:CB	2:D:348:LEU:HD22	2.50	0.41
1:A:199:ARG:CZ	1:A:199:ARG:HB2	2.49	0.41
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.80	0.41
2:D:230:GLU:HG3	2:D:268:GLU:HG2	2.02	0.41
1:A:197:VAL:HG11	1:A:252:VAL:HG12	2.02	0.41
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.94	0.41
2:B:282:THR:O	2:B:285:THR:OG1	2.35	0.41
2:B:411:GLU:HG2	2:B:411:GLU:H	1.66	0.41
1:C:75:LYS:HE3	1:C:75:LYS:HB2	1.97	0.40
1:C:194:ALA:CB	1:C:202:LEU:HD22	2.51	0.40
2:D:199:TYR:CD1	2:D:199:TYR:C	2.99	0.40
1:A:94:SER:O	1:A:98:GLY:N	2.50	0.40
1:A:194:ALA:CB	1:A:202:LEU:HD22	2.52	0.40
1:C:6:LYS:HD3	1:C:19:TYR:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/302 (95%)	277 (96%)	10 (4%)	1 (0%)	36	46
1	C	293/302 (97%)	268 (92%)	22 (8%)	3 (1%)	12	15
2	B	255/260 (98%)	250 (98%)	5 (2%)	0	100	100
2	D	253/260 (97%)	242 (96%)	10 (4%)	1 (0%)	30	38
All	All	1089/1124 (97%)	1037 (95%)	47 (4%)	5 (0%)	24	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	C	167	TRP
1	A	164	VAL
1	C	40	GLU
2	D	372	TRP

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	257/264 (97%)	230 (90%)	27 (10%)	6	8
1	C	260/264 (98%)	230 (88%)	30 (12%)	5	6
2	B	231/234 (99%)	219 (95%)	12 (5%)	21	31
2	D	229/234 (98%)	215 (94%)	14 (6%)	17	24
All	All	977/996 (98%)	894 (92%)	83 (8%)	10	13

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	12	GLU
1	A	36	ARG
1	A	41	THR
1	A	55	LEU
1	A	59	ASN
1	A	73	GLU
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	88	LYS
1	A	97	THR
1	A	101	LEU
1	A	143	LEU
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL

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Mol	Chain	Res	Type
1	A	178	LYS
1	A	184	VAL
1	A	189	LEU
1	A	199	ARG
1	A	200	ARG
1	A	206	ASP
1	A	226	VAL
1	A	230	VAL
1	A	237	LYS
1	A	255	LEU
2	B	176	PRO
2	B	180	GLU
2	B	196	LYS
2	B	232	LEU
2	B	281	ILE
2	B	292	LEU
2	B	316	THR
2	B	323	GLN
2	B	328	LYS
2	B	348	LEU
2	B	374	GLU
2	B	384	LEU
1	C	0	SER
1	C	9	LYS
1	C	14	THR
1	C	24	LYS
1	C	46	SER
1	C	55	LEU
1	C	74	ASN
1	C	75	LYS
1	C	76	LEU
1	C	78	LEU
1	C	88	LYS
1	C	97	THR
1	C	101	LEU
1	C	148	LEU
1	C	150	ARG
1	C	154	VAL
1	C	157	ARG
1	C	163	VAL
1	C	164	VAL
1	C	175	LEU

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Mol	Chain	Res	Type
1	C	197	VAL
1	C	200	ARG
1	C	206	ASP
1	C	209	ILE
1	C	217	ARG
1	C	230	VAL
1	C	231	THR
1	C	255	LEU
1	C	278	LYS
1	C	295	HIS
2	D	180	GLU
2	D	189	MET
2	D	201	LYS
2	D	232	LEU
2	D	281	ILE
2	D	292	LEU
2	D	316	THR
2	D	348	LEU
2	D	384	LEU
2	D	391	LEU
2	D	409	ILE
2	D	428	GLU
2	D	431	ASN
2	D	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	74	ASN
1	A	84	HIS
1	A	119	HIS
1	A	265	GLN
1	A	268	HIS
2	B	228	GLN
2	B	254	GLN
2	B	296	HIS
2	B	370	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN

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Mol	Chain	Res	Type
1	C	3	ASN
1	C	60	HIS
1	C	74	ASN
1	C	84	HIS
1	C	113	GLN
1	C	119	HIS
1	C	265	GLN
1	C	268	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	361	HIS
2	D	395	HIS
2	D	406	GLN
2	D	431	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	A	160	1	8,10,11	0.93	0	10,14,16	1.17	1 (10%)
1	TPO	C	160	1	8,10,11	1.01	1 (12%)	10,14,16	1.12	1 (10%)

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	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	2.23	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O3P-P-O2P	2.34	116.56	107.80
1	C	160	TPO	O-C-CA	-2.06	119.48	124.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB

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	QQ2	C	1296	-	35,35,35	1.02	3 (8%)	44,47,47	2.14	10 (22%)
3	QQ2	A	1296	-	35,35,35	1.14	3 (8%)	44,47,47	2.45	15 (34%)
4	SGM	B	1433	2	5,5,5	1.01	0	5,5,5	0.78	0
4	SGM	D	1433	-	5,5,5	0.45	0	5,5,5	0.57	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	QQ2	C	1296	-	-	9/23/24/24	0/3/3/3
3	QQ2	A	1296	-	-	3/23/24/24	0/3/3/3
4	SGM	B	1433	2	-	1/4/4/4	-
4	SGM	D	1433	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1296	QQ2	C8-N7	-2.78	1.38	1.43
3	C	1296	QQ2	C13-CL1	2.59	1.79	1.73
3	A	1296	QQ2	C8-N7	-2.51	1.38	1.43
3	C	1296	QQ2	C20-N19	-2.41	1.35	1.40
3	A	1296	QQ2	C16-C17	2.27	1.50	1.47
3	A	1296	QQ2	C5-N19	2.19	1.42	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1296	QQ2	C1-N2-C3	8.21	121.84	114.95
3	A	1296	QQ2	C1-N2-C3	7.44	121.19	114.95
3	A	1296	QQ2	C5-C4-C3	5.45	121.00	116.64
3	C	1296	QQ2	N6-C1-N2	-4.90	121.16	128.58
3	A	1296	QQ2	O26-C27-C28	4.82	116.33	107.64
3	A	1296	QQ2	C32-N30-C29	4.62	122.91	111.00
3	A	1296	QQ2	C4-C5-N6	-3.82	117.91	122.92
3	A	1296	QQ2	N6-C1-N2	-3.77	122.87	128.58
3	A	1296	QQ2	C4-C3-N2	-3.69	116.68	122.82
3	C	1296	QQ2	C16-C17-N18	-3.66	172.83	177.91
3	A	1296	QQ2	C31-N30-C29	3.59	120.26	111.00
3	C	1296	QQ2	C32-N30-C31	3.46	118.60	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1296	QQ2	C13-C8-N7	3.44	123.97	121.03
3	C	1296	QQ2	C32-N30-C29	2.76	118.12	111.00
3	A	1296	QQ2	C27-O26-C23	2.74	123.89	117.85
3	C	1296	QQ2	C13-C8-N7	2.69	123.33	121.03
3	C	1296	QQ2	C4-C3-N2	-2.65	118.42	122.82
3	A	1296	QQ2	C32-N30-C31	2.61	116.41	109.72
3	A	1296	QQ2	C29-C28-C27	2.53	117.24	111.59
3	C	1296	QQ2	C4-C5-N6	-2.49	119.65	122.92
3	A	1296	QQ2	C21-C22-C23	2.31	122.37	119.73
3	A	1296	QQ2	C8-C13-CL1	2.10	122.56	120.24
3	C	1296	QQ2	O33-C28-C29	2.08	115.90	109.91
3	A	1296	QQ2	C11-C10-C9	2.07	121.01	117.96
3	C	1296	QQ2	C4-C3-N7	2.06	124.80	122.13

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1296	QQ2	O26-C27-C28-C29
3	C	1296	QQ2	O26-C27-C28-C29
3	C	1296	QQ2	C27-C28-C29-N30
4	D	1433	SGM	S1-C1-C2-C3
4	D	1433	SGM	C1-C2-C3-O3
3	C	1296	QQ2	C24-C23-O26-C27
3	C	1296	QQ2	C22-C23-O26-C27
3	A	1296	QQ2	O26-C27-C28-O33
3	C	1296	QQ2	O26-C27-C28-O33
4	D	1433	SGM	O2-C2-C3-O3
4	B	1433	SGM	S1-C1-C2-O2
3	C	1296	QQ2	O33-C28-C29-N30
3	A	1296	QQ2	C28-C29-N30-C31
3	C	1296	QQ2	C28-C27-O26-C23
3	C	1296	QQ2	C28-C29-N30-C31
3	C	1296	QQ2	C28-C29-N30-C32

There are no ring outliers.

3 monomers are involved in 10 short contacts:

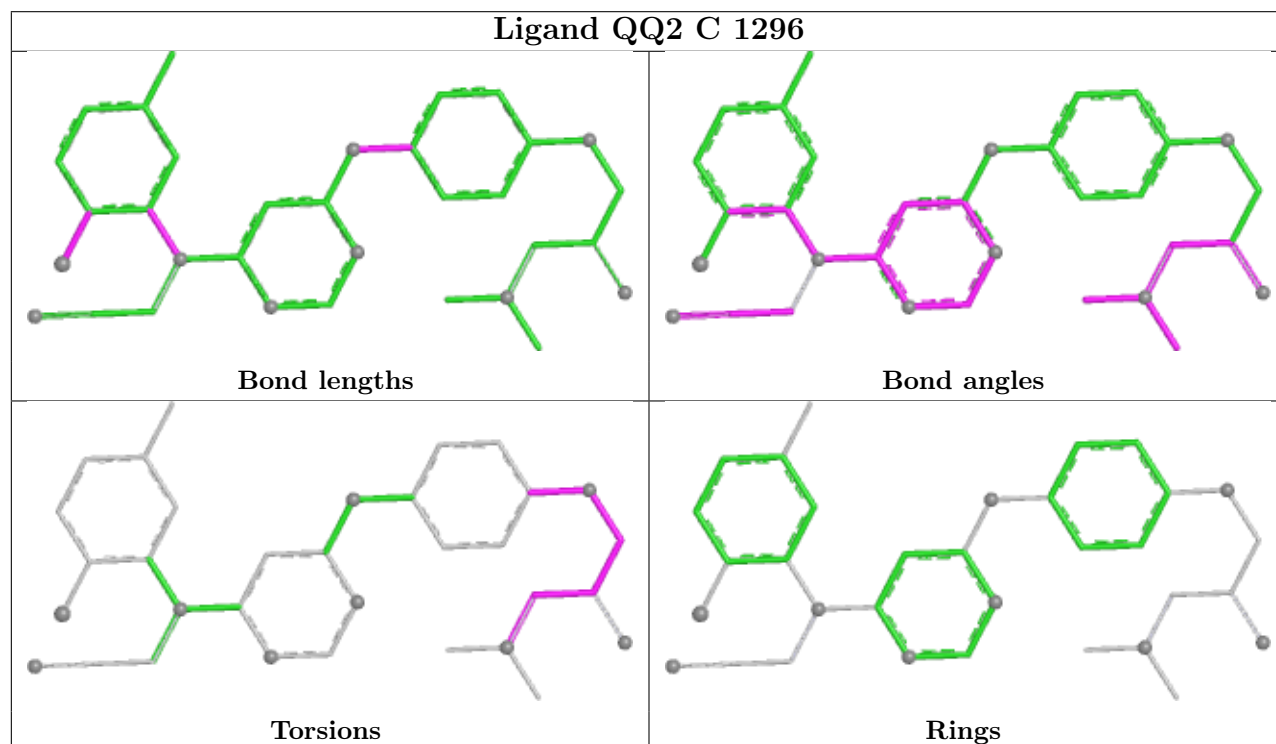
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1296	QQ2	5	0
3	A	1296	QQ2	4	0

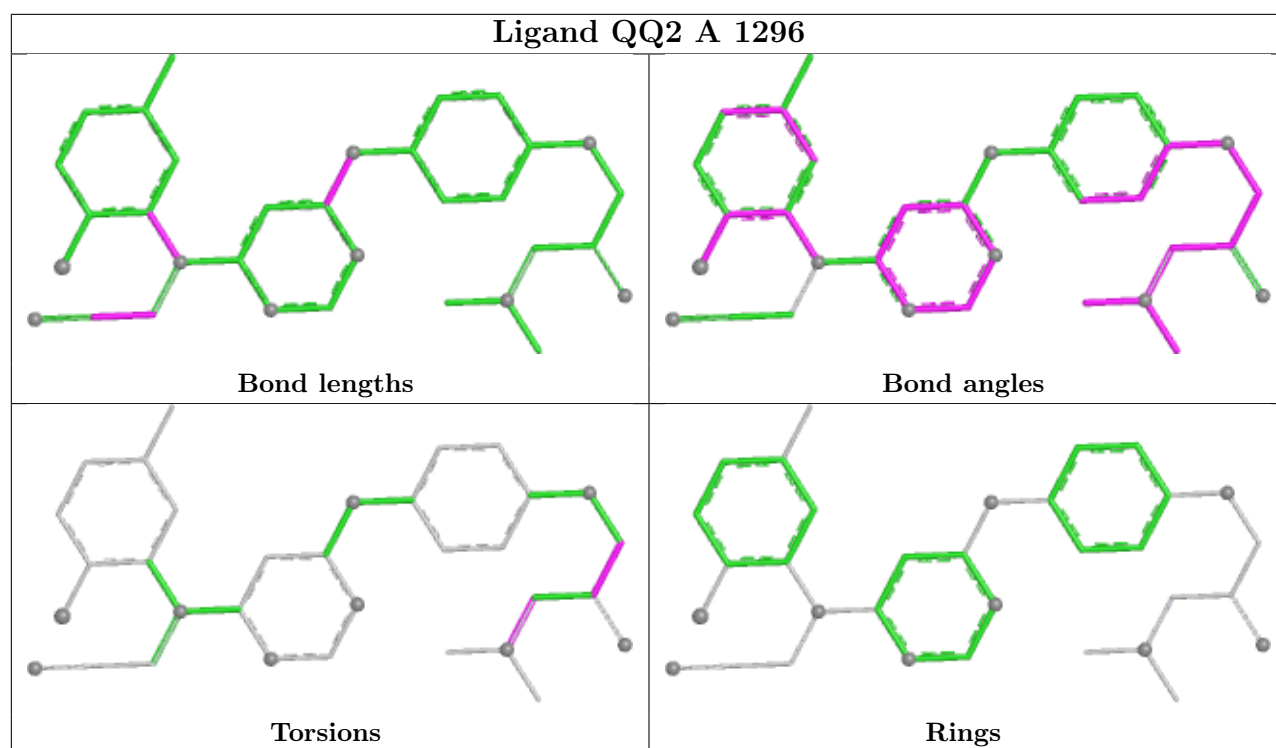
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1433	SGM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	292/302 (96%)	1.25	37 (12%)	8 8	26, 35, 46, 59	0
1	C	295/302 (97%)	1.52	79 (26%)	1 1	24, 35, 45, 58	0
2	B	257/260 (98%)	1.09	23 (8%)	15 17	29, 35, 44, 52	0
2	D	255/260 (98%)	1.55	72 (28%)	1 1	30, 36, 43, 48	0
All	All	1099/1124 (97%)	1.35	211 (19%)	3 3	24, 35, 45, 59	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	THR	6.8
1	A	14	THR	6.4
2	D	430	LEU	5.5
1	A	15	TYR	5.3
1	A	13	GLY	5.3
1	A	96	LEU	5.2
1	C	229	GLY	5.1
2	D	367	VAL	5.0
1	C	226	VAL	4.6
2	B	284	ASP	4.6
1	C	225	VAL	4.6
1	C	295	HIS	4.5
1	C	243	TRP	4.4
1	A	295	HIS	4.3
1	A	73	GLU	4.2
2	D	326	ASN	4.2
1	C	233	MET	4.2
1	A	72	THR	4.2
1	C	236	TYR	4.2
1	A	17	VAL	4.1
2	D	369	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	372	TRP	4.0
1	C	227	TRP	3.9
1	C	234	PRO	3.9
2	D	392	MET	3.9
1	A	12	GLU	3.7
2	D	426	PRO	3.7
1	C	203	PHE	3.7
1	C	17	VAL	3.7
2	D	368	THR	3.7
2	B	176	PRO	3.7
2	D	418	TYR	3.7
2	D	365	TYR	3.7
1	C	238	PRO	3.7
2	B	201	LYS	3.7
2	B	323	GLN	3.6
2	D	399	LEU	3.6
2	D	371	SER	3.6
1	A	162	GLU	3.6
1	A	71	HIS	3.6
2	D	402	PRO	3.5
1	A	94	SER	3.5
2	D	419	HIS	3.5
1	C	223	ASP	3.5
2	B	280	TYR	3.5
1	A	256	ASP	3.5
1	C	240	PHE	3.5
2	D	401	ALA	3.4
2	D	350	TYR	3.4
1	C	241	PRO	3.4
2	D	395	HIS	3.4
1	C	16	GLY	3.4
1	C	213	PHE	3.4
1	C	217	ARG	3.4
2	D	333	ALA	3.4
1	A	95	ALA	3.3
1	C	232	SER	3.3
1	C	247	ASP	3.3
1	C	246	GLN	3.3
1	C	202	LEU	3.2
2	D	384	LEU	3.2
1	A	206	ASP	3.2
2	D	429	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	235	ASP	3.2
2	D	385	GLU	3.2
1	C	219	LEU	3.2
1	C	209	ILE	3.1
1	A	19	TYR	3.1
1	C	215	ILE	3.0
1	C	187	TRP	3.0
1	A	0	SER	3.0
1	C	256	ASP	3.0
2	B	198	GLY	3.0
2	B	324	PRO	3.0
1	C	96	LEU	3.0
2	B	296	HIS	2.9
2	D	327	CYS	2.9
1	C	231	THR	2.9
1	C	175	LEU	2.9
1	C	244	ALA	2.9
1	C	255	LEU	2.9
1	C	271	PRO	2.9
2	B	385	GLU	2.9
1	C	39	THR	2.9
1	C	277	ALA	2.8
2	D	325	ALA	2.8
1	C	173	ILE	2.8
2	D	390	CYS	2.8
1	C	15	TYR	2.8
1	C	252	VAL	2.8
2	D	300	LYS	2.8
2	B	283	ASP	2.8
2	D	322	GLN	2.8
1	C	99	ILE	2.7
2	D	324	PRO	2.7
1	A	293	VAL	2.7
2	D	375	SER	2.7
1	C	171	PRO	2.7
2	D	329	VAL	2.7
2	D	397	THR	2.7
1	A	93	ALA	2.6
1	C	269	TYR	2.6
1	A	59	ASN	2.6
1	C	228	PRO	2.6
1	A	258	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	396	GLN	2.6
2	D	357	GLY	2.6
2	D	366	THR	2.6
2	D	363	ALA	2.5
1	C	248	PHE	2.5
1	A	84	HIS	2.5
1	C	273	LYS	2.5
1	A	179	TYR	2.5
2	B	196	LYS	2.5
1	A	164	VAL	2.5
1	C	95	ALA	2.5
1	C	258	ASP	2.5
1	C	254	PRO	2.5
1	C	259	GLY	2.5
1	C	249	SER	2.5
1	C	179	TYR	2.5
2	B	432	LEU	2.5
2	D	432	LEU	2.5
1	A	74	ASN	2.5
1	C	210	ASP	2.5
2	D	320	LEU	2.4
1	A	2	GLU	2.4
1	C	13	GLY	2.4
1	C	253	PRO	2.4
1	A	97	THR	2.4
1	C	221	THR	2.4
2	D	347	TYR	2.4
2	D	361	HIS	2.4
2	D	312	ASN	2.4
1	A	8	GLU	2.4
2	D	416	SER	2.4
1	A	10	ILE	2.4
1	C	286	PHE	2.4
2	B	289	LYS	2.4
1	C	163	VAL	2.4
2	D	311	VAL	2.4
2	D	388	LYS	2.4
1	A	251	VAL	2.4
2	D	409	ILE	2.4
2	D	376	LEU	2.4
1	C	288	ASP	2.3
2	D	229	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	192	ILE	2.3
2	D	428	GLU	2.3
2	B	431	ASN	2.3
2	D	382	TYR	2.3
2	D	378	ARG	2.3
2	B	428	GLU	2.3
2	D	256	VAL	2.3
2	D	431	ASN	2.3
1	C	153	GLY	2.3
2	D	381	GLY	2.3
2	D	413	TYR	2.3
1	C	0	SER	2.3
1	C	237	LYS	2.3
1	C	242	LYS	2.3
2	D	364	LEU	2.3
2	D	391	LEU	2.3
1	C	200	ARG	2.3
2	D	427	PRO	2.2
2	B	274	GLU	2.2
1	C	197	VAL	2.2
1	C	230	VAL	2.2
2	D	314	PHE	2.2
2	B	220	GLU	2.2
1	C	35	ILE	2.2
2	D	377	ILE	2.2
1	A	37	LEU	2.2
2	D	332	LEU	2.2
2	B	402	PRO	2.2
1	A	287	GLN	2.2
2	D	400	LYS	2.2
2	B	325	ALA	2.2
1	C	46	SER	2.2
1	C	207	SER	2.2
2	D	310	THR	2.2
1	C	245	ARG	2.2
1	A	41	THR	2.2
1	A	32	LEU	2.1
1	C	275	ILE	2.1
1	C	251	VAL	2.1
1	C	289	VAL	2.1
1	C	257	GLU	2.1
1	A	16	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	331	SER	2.1
1	A	35	ILE	2.1
1	C	262	LEU	2.1
2	B	281	ILE	2.1
2	D	348	LEU	2.1
1	C	64	VAL	2.1
2	B	352	PRO	2.1
2	D	323	GLN	2.1
2	D	425	ASN	2.1
1	C	218	THR	2.1
2	B	193	CYS	2.1
2	D	417	LYS	2.1
1	A	148	LEU	2.1
1	C	74	ASN	2.1
2	D	398	TYR	2.1
2	D	360	PHE	2.1
2	D	244	SER	2.0
2	D	386	SER	2.0
2	B	374	GLU	2.0
2	D	334	MET	2.0
2	D	403	GLN	2.0
2	D	373	PRO	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($\text{\AA}^2$)	Q<0.9
1	TPO	C	160	11/12	0.92	0.10	31,33,36,36	0
1	TPO	A	160	11/12	0.98	0.09	29,32,34,34	0

6.3 Carbohydrates [i](#)

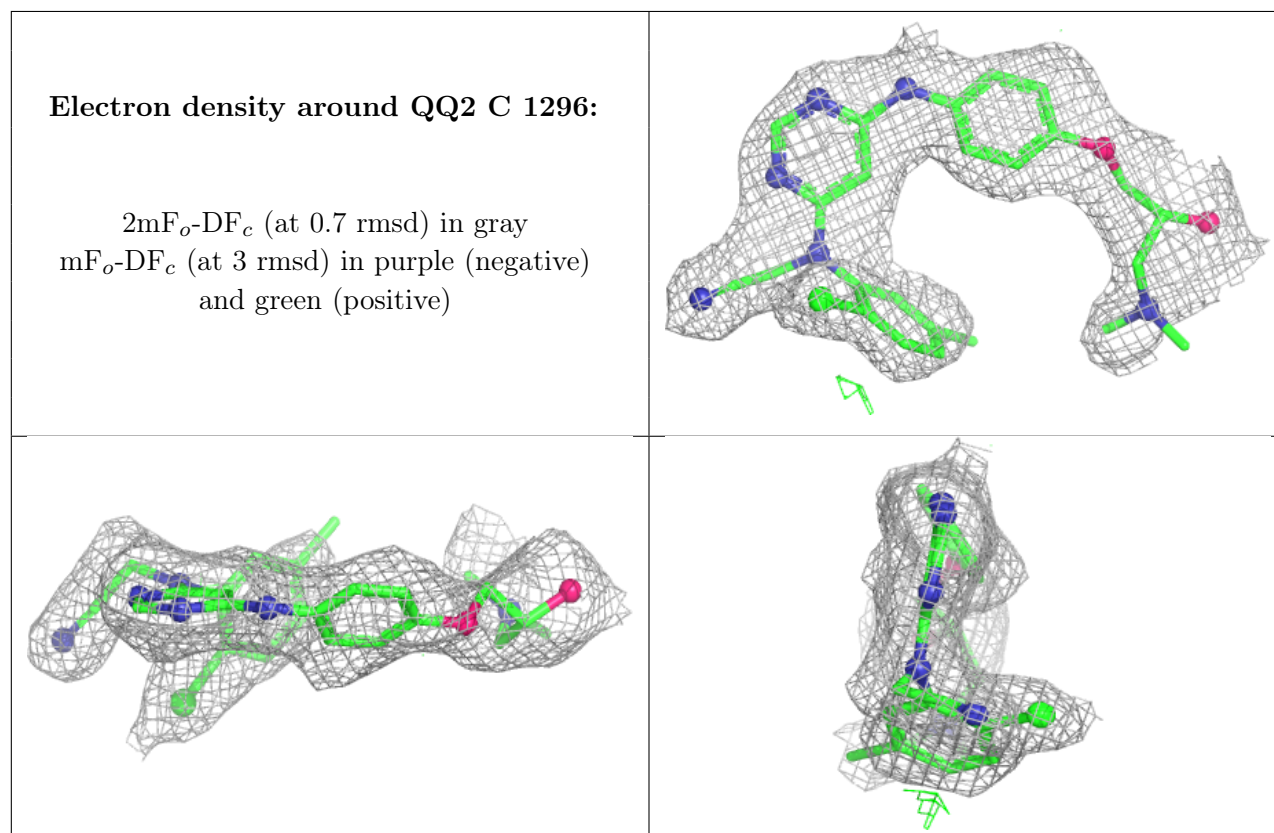
There are no oligosaccharides in this entry.

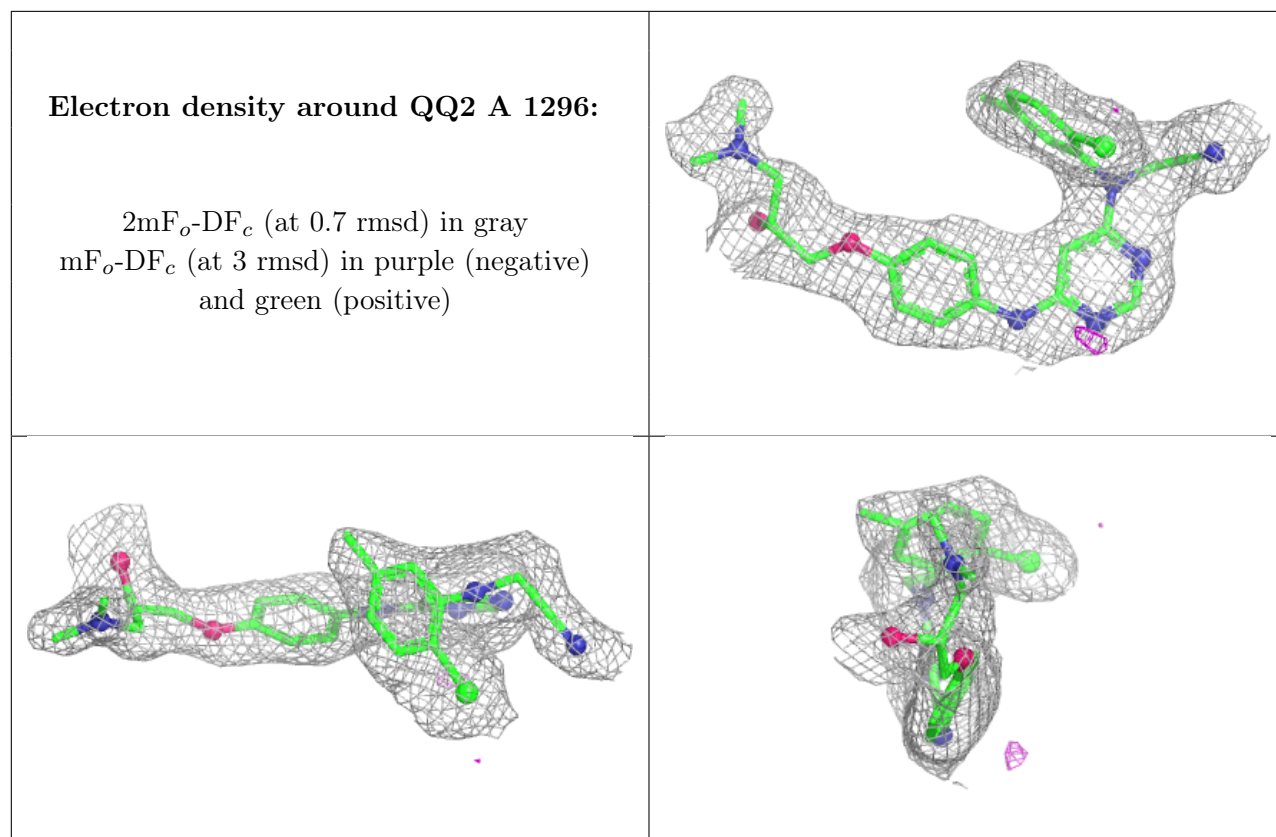
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	QQ2	C	1296	33/33	0.80	0.16	40,44,54,56	0
3	QQ2	A	1296	33/33	0.85	0.16	35,45,54,56	0
4	SGM	D	1433	6/6	0.87	0.16	54,55,55,56	0
4	SGM	B	1433	6/6	0.88	0.14	42,45,48,50	0
5	MG	B	1434	1/1	0.90	0.10	31,31,31,31	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.