



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:22 pm BST

PDB ID : 2IW6
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

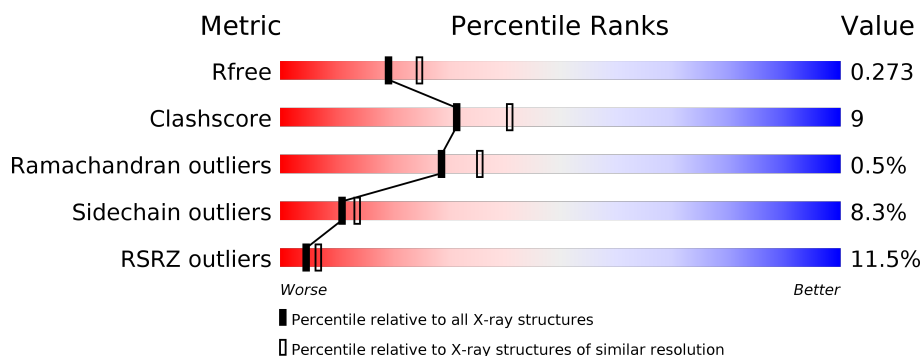
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	
1	C	302	
2	B	260	
2	D	260	

2 Entry composition

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

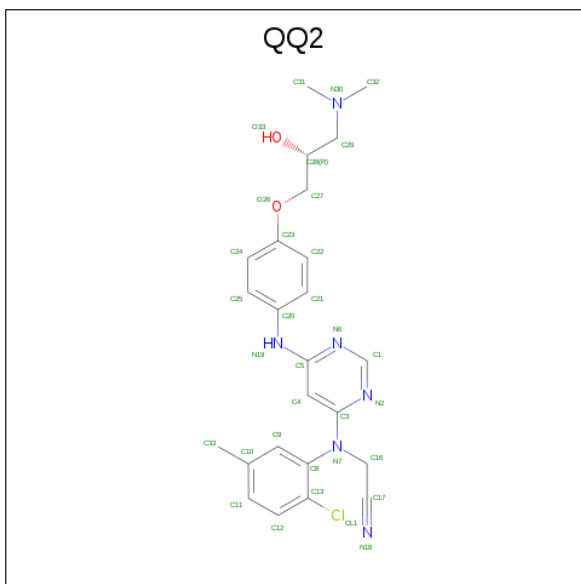
- Molecule 2 is a protein called CYCLIN-A2.

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:

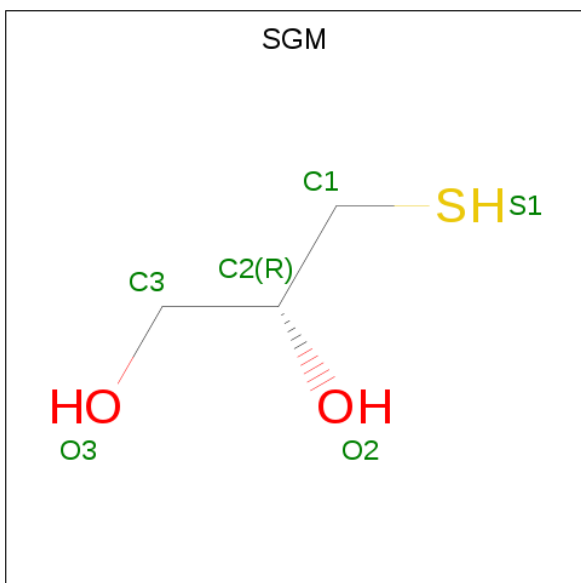
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	expression tag	UNP P20248
D	173	MET	-	expression tag	UNP P20248

- Molecule 3 is [(2-CHLORO-5-METHYLPHENYL){6-[(4-{[(2R)-3-(DIMETHYLAMINO)-2-HYDROXYPROPYL]OXY}PHENYL)AMINO]PYRIMIDIN-4-YL}AMINO]ACETONITRILE (three-letter code: QQ2) (formula: C₂₄H₂₇ClN₆O₂).



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

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: C₃H₈O₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			6	3	2	1		
4	D	1	Total	C	O	S	0	0
			6	3	2	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

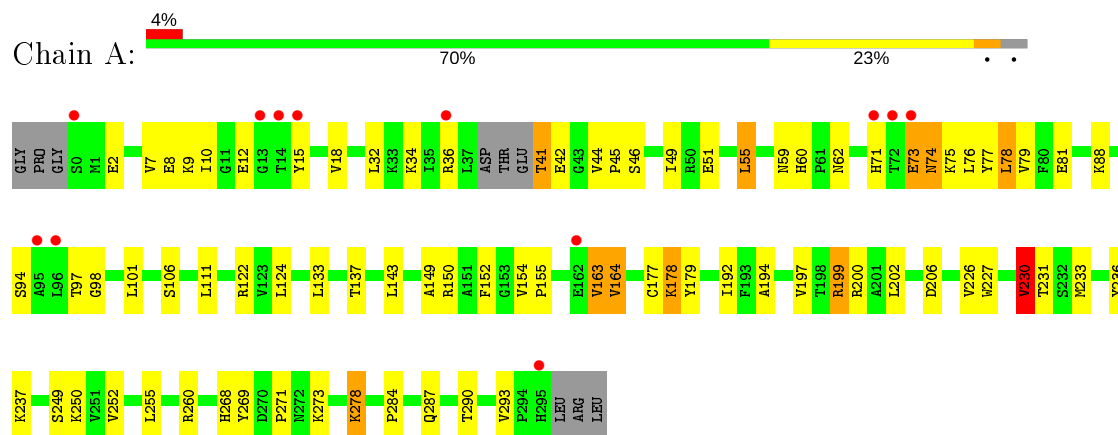
- Molecule 6 is water.

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		

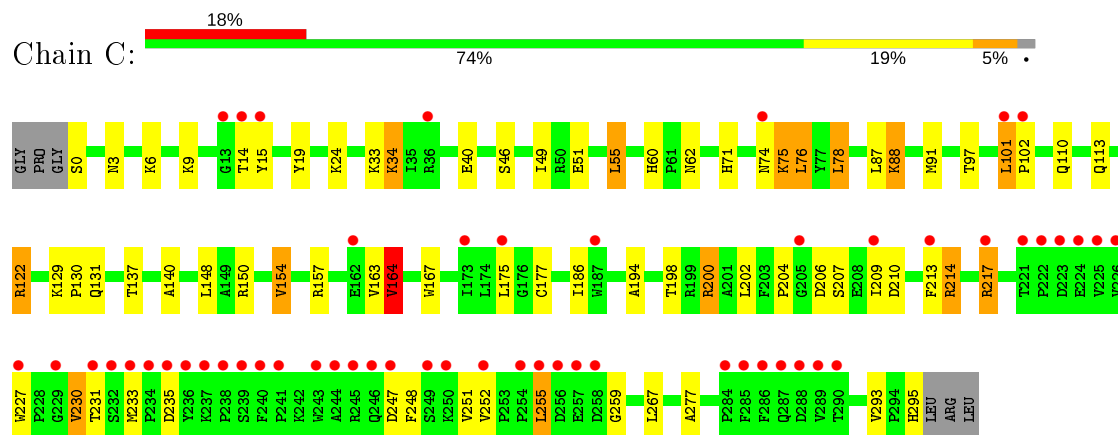
3 Residue-property plots [i](#)

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

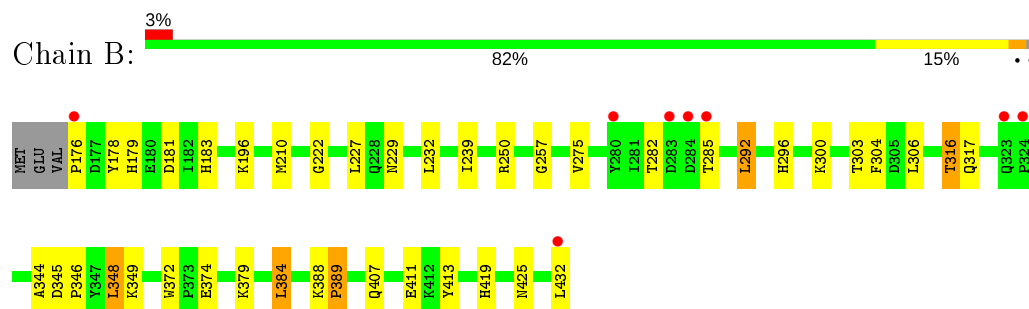
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



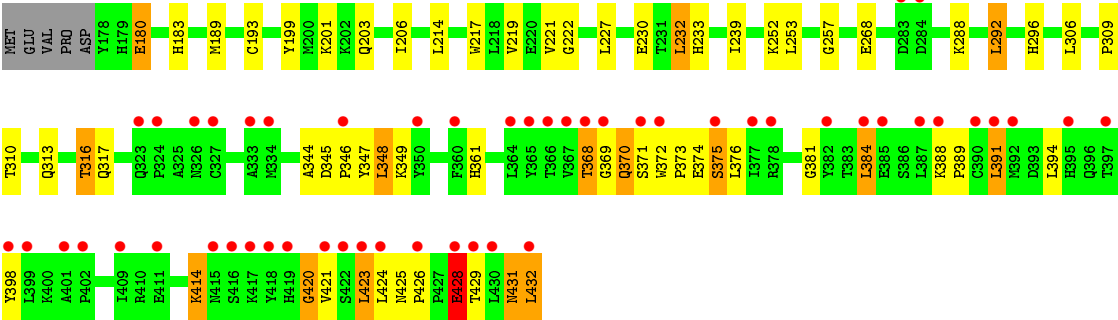
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 2: CYCLIN-A2



● Molecule 2: CYCLIN-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.78Å 134.56Å 148.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 41.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.1 (100.00-2.30) 92.7 (41.06-2.30)	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)	0.33 , 49.5	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	0.94	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, MG, SGM, 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	0.83	0/2403	0.88	2/3260 (0.1%)
1	C	0.63	0/2428	0.74	2/3296 (0.1%)
2	B	0.79	1/2126 (0.0%)	0.83	0/2886
2	D	1.23	26/2110 (1.2%)	0.82	2/2864 (0.1%)
All	All	0.89	27/9067 (0.3%)	0.82	6/12306 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	375	SER	CB-OG	19.35	1.67	1.42
2	D	423	LEU	C-O	13.67	1.49	1.23
2	D	370	GLN	CD-OE1	10.37	1.46	1.24
2	D	429	THR	C-N	9.75	1.56	1.34
2	D	374	GLU	CD-OE2	9.52	1.36	1.25
2	D	420	GLY	C-N	8.78	1.54	1.34
2	D	414	LYS	CE-NZ	8.67	1.70	1.49
2	D	425	ASN	CG-ND2	8.61	1.54	1.32
2	D	421	VAL	C-N	8.25	1.53	1.34
2	D	425	ASN	CG-OD1	8.20	1.42	1.24
2	D	421	VAL	C-O	7.76	1.38	1.23
2	D	423	LEU	C-N	7.27	1.50	1.34
2	D	428	GLU	CD-OE1	-7.10	1.17	1.25
2	D	420	GLY	C-O	6.73	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	381	GLY	C-N	6.65	1.49	1.34
2	D	381	GLY	C-O	6.51	1.34	1.23
2	D	428	GLU	CA-CB	6.50	1.68	1.53
2	D	368	THR	CB-OG1	6.42	1.56	1.43
2	D	369	GLY	C-N	6.24	1.48	1.34
2	D	428	GLU	C-O	-5.96	1.12	1.23
2	D	426	PRO	N-CD	5.95	1.56	1.47
2	D	424	LEU	CG-CD2	5.85	1.73	1.51
2	D	429	THR	CB-OG1	5.25	1.53	1.43
2	B	178	TYR	CD1-CE1	-5.20	1.31	1.39
2	D	371	SER	CB-OG	5.15	1.49	1.42
2	D	370	GLN	C-O	5.15	1.33	1.23
2	D	431	ASN	C-O	5.08	1.33	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	LEU	CA-CB-CG	5.83	128.71	115.30
2	D	423	LEU	O-C-N	5.74	131.89	122.70
1	A	230	VAL	CB-CA-C	-5.67	100.63	111.40
1	A	78	LEU	CA-CB-CG	5.33	127.56	115.30
2	D	429	THR	CA-C-N	-5.31	105.52	117.20
1	C	122	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	57	0
1	C	2378	0	2413	41	0
2	B	2076	0	2098	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2061	0	2086	38	0
3	A	33	0	27	4	0
3	C	33	0	27	4	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	162	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 (162) 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: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:HG2	1:C:200:ARG:HH11	1.23	1.03
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.48	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
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:C:177:CYS:HB2	1:C:233:MET:CE	2.08	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:C:177:CYS:HB2	1:C:233:MET:HE2	1.68	0.75
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:O	2:B:316:THR:HG22	1.89	0.72
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
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
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.82	0.61
1:C:177:CYS:HB2	1:C:233:MET:HE3	1.81	0.60
2:B:229:ASN:HD22	2:B:334:MET:CE	2.14	0.60
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
2:B:229:ASN:HD22	2:B:334:MET:HE2	1.68	0.58
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
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:N	1:A:74:ASN:HD22	2.04	0.55
1:A:41:THR:HG22	1:A:42:GLU:H	1.72	0.55
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:A:60:HIS:CD2	1:A:62:ASN:H	2.25	0.54
2:D:375:SER:HG	2:D:375:SER:CB	2.10	0.53
2:D:180:GLU:OE1	2:D:180:GLU:HA	2.08	0.53
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.96	0.53
2:D:368:THR:OG1	2:D:370:GLN:HG3	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:373:PRO:HD2	2:D:376:LEU:HD12	1.90	0.53
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:C21	3:C:1296:QQ2:H4	2.41	0.50
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.47	0.49
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.93	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:177:CYS:HB2	1:A:233:MET:HE2	1.95	0.47
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.95	0.47
1:A:15:TYR:N	1:A:15:TYR:CD1	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:CG	1:C:200:ARG:HH11	2.09	0.47
1:A:249:SER:HA	1:A:260:ARG:HD3	1.96	0.47
3:C:1296:QQ2:C4	3:C:1296:QQ2:C21	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:C:34:LYS:HE3	1:C:75:LYS:HZ3	1.80	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:HB3	2:B:389:PRO:CD	2.47	0.45
1:C:163:VAL:HG12	1:C:164:VAL:HG23	1.99	0.45
1:C:51:GLU:O	1:C:55:LEU:HB2	2.16	0.45
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.05	0.45
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:A:178:LYS:HE2	1:A:178:LYS:HB2	1.93	0.43
1:A:106:SER:HB2	1:A:290:THR:O	2.18	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:HA	2:B:425:ASN:HD22	1.67	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
3:A:1296:QQ2:C4	3:A:1296:QQ2:H21	2.50	0.41
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.50	0.41
2:D:233:HIS:HB3	2:D:310:THR:HB	2.01	0.41
2:D:206:ILE:HD13	2:D:253:LEU:HD13	2.03	0.41
1:A:81:GLU:HG3	1:A:81:GLU:O	2.19	0.41
1:C:110:GLN:OE1	1:C:140:ALA:HA	2.20	0.41

Continued on next page...

Continued from previous page...

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:HB2	1:A:199:ARG:CZ	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:H	2:B:411:GLU:HG2	1.66	0.41
1:C:194:ALA:CB	1:C:202:LEU:HD22	2.51	0.40
1:C:75:LYS:HE3	1:C:75:LYS:HB2	1.97	0.40
1:A:194:ALA:CB	1:A:202:LEU:HD22	2.52	0.40
1:A:94:SER:O	1:A:98:GLY:N	2.50	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 [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	288/302 (95%)	277 (96%)	10 (4%)	1 (0%)	41	50
1	C	293/302 (97%)	268 (92%)	22 (8%)	3 (1%)	15	17
2	B	255/260 (98%)	250 (98%)	5 (2%)	0	100	100
2	D	253/260 (97%)	242 (96%)	10 (4%)	1 (0%)	34	42
All	All	1089/1124 (97%)	1037 (95%)	47 (4%)	5 (0%)	29	35

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%)	7	8
1	C	260/264 (98%)	230 (88%)	30 (12%)	5	6
2	B	231/234 (99%)	221 (96%)	10 (4%)	29	40
2	D	229/234 (98%)	215 (94%)	14 (6%)	18	25
All	All	977/996 (98%)	896 (92%)	81 (8%)	11	14

All (81) 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	46	SER
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	122	ARG
1	A	143	LEU
1	A	150	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	163	VAL
1	A	178	LYS
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
1	A	278	LYS
2	B	176	PRO
2	B	196	LYS
2	B	232	LEU
2	B	292	LEU
2	B	300	LYS
2	B	316	THR
2	B	348	LEU
2	B	374	GLU
2	B	384	LEU
2	B	389	PRO
1	C	0	SER
1	C	9	LYS
1	C	14	THR
1	C	34	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	122	ARG
1	C	148	LEU
1	C	150	ARG
1	C	154	VAL
1	C	157	ARG
1	C	164	VAL
1	C	200	ARG
1	C	206	ASP
1	C	209	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	214	ARG
1	C	217	ARG
1	C	230	VAL
1	C	231	THR
1	C	247	ASP
1	C	248	PHE
1	C	255	LEU
1	C	295	HIS
2	D	180	GLU
2	D	189	MET
2	D	199	TYR
2	D	201	LYS
2	D	232	LEU
2	D	292	LEU
2	D	316	THR
2	D	348	LEU
2	D	384	LEU
2	D	391	LEU
2	D	398	TYR
2	D	428	GLU
2	D	431	ASN
2	D	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	74	ASN
1	A	119	HIS
1	A	265	GLN
1	A	268	HIS
2	B	254	GLN
2	B	296	HIS
2	B	370	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
1	C	59	ASN
1	C	60	HIS
1	C	84	HIS
1	C	113	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	119	HIS
1	C	121	HIS
1	C	268	HIS
2	D	179	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	361	HIS
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	0.90	0	10,14,16	1.14	1 (10%)
1	TPO	C	160	1	8,10,11	0.99	1 (12%)	10,14,16	1.10	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	2.18	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	160	TPO	O3P-P-O2P	2.34	116.56	107.64
1	C	160	TPO	O-C-CA	-2.02	119.48	124.78

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 carbohydrates 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	$\# Z > 2$
4	SGM	D	1433	-	5,5,5	0.44	0	5,5,5	0.56	0
3	QQ2	C	1296	-	35,35,35	1.00	4 (11%)	41,47,47	2.09	9 (21%)
3	QQ2	A	1296	-	35,35,35	1.12	3 (8%)	41,47,47	2.26	13 (31%)
4	SGM	B	1433	2	5,5,5	0.98	0	5,5,5	0.75	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
4	SGM	D	1433	-	-	3/4/4/4	-
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	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1296	QQ2	C13-CL1	2.57	1.79	1.73
3	C	1296	QQ2	C8-N7	-2.42	1.38	1.43
3	A	1296	QQ2	C16-C17	2.41	1.50	1.47
3	C	1296	QQ2	C20-N19	-2.33	1.35	1.40
3	A	1296	QQ2	C5-N19	2.20	1.42	1.38
3	A	1296	QQ2	C8-N7	-2.19	1.38	1.43
3	C	1296	QQ2	C3-N7	-2.01	1.36	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1296	QQ2	C1-N2-C3	7.90	121.84	114.94
3	A	1296	QQ2	C1-N2-C3	7.16	121.19	114.94
3	C	1296	QQ2	N6-C1-N2	-4.76	121.16	128.60
3	A	1296	QQ2	O26-C27-C28	4.67	116.33	107.63
3	A	1296	QQ2	C32-N30-C29	4.53	122.91	111.01
3	C	1296	QQ2	C16-C17-N18	-3.68	172.83	177.90
3	A	1296	QQ2	N6-C1-N2	-3.67	122.87	128.60
3	A	1296	QQ2	C31-N30-C29	3.52	120.26	111.01
3	A	1296	QQ2	C4-C3-N2	-3.49	116.68	122.73
3	A	1296	QQ2	C4-C5-N6	-3.47	117.91	122.75
3	C	1296	QQ2	C32-N30-C31	3.43	118.60	109.73
3	A	1296	QQ2	C27-O26-C23	2.81	123.89	117.93
3	C	1296	QQ2	C32-N30-C29	2.71	118.12	111.01
3	A	1296	QQ2	C32-N30-C31	2.58	116.41	109.73
3	A	1296	QQ2	C29-C28-C27	2.49	117.24	111.72
3	C	1296	QQ2	C4-C3-N2	-2.49	118.42	122.73
3	A	1296	QQ2	C8-C13-CL1	2.24	122.56	120.22
3	C	1296	QQ2	C4-C5-N6	-2.22	119.65	122.75
3	A	1296	QQ2	C21-C22-C23	2.15	122.37	119.73
3	C	1296	QQ2	O33-C28-C29	2.10	115.90	109.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1296	QQ2	C4-C3-N7	2.05	124.80	122.18
3	A	1296	QQ2	C11-C10-C9	2.03	121.01	117.95

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

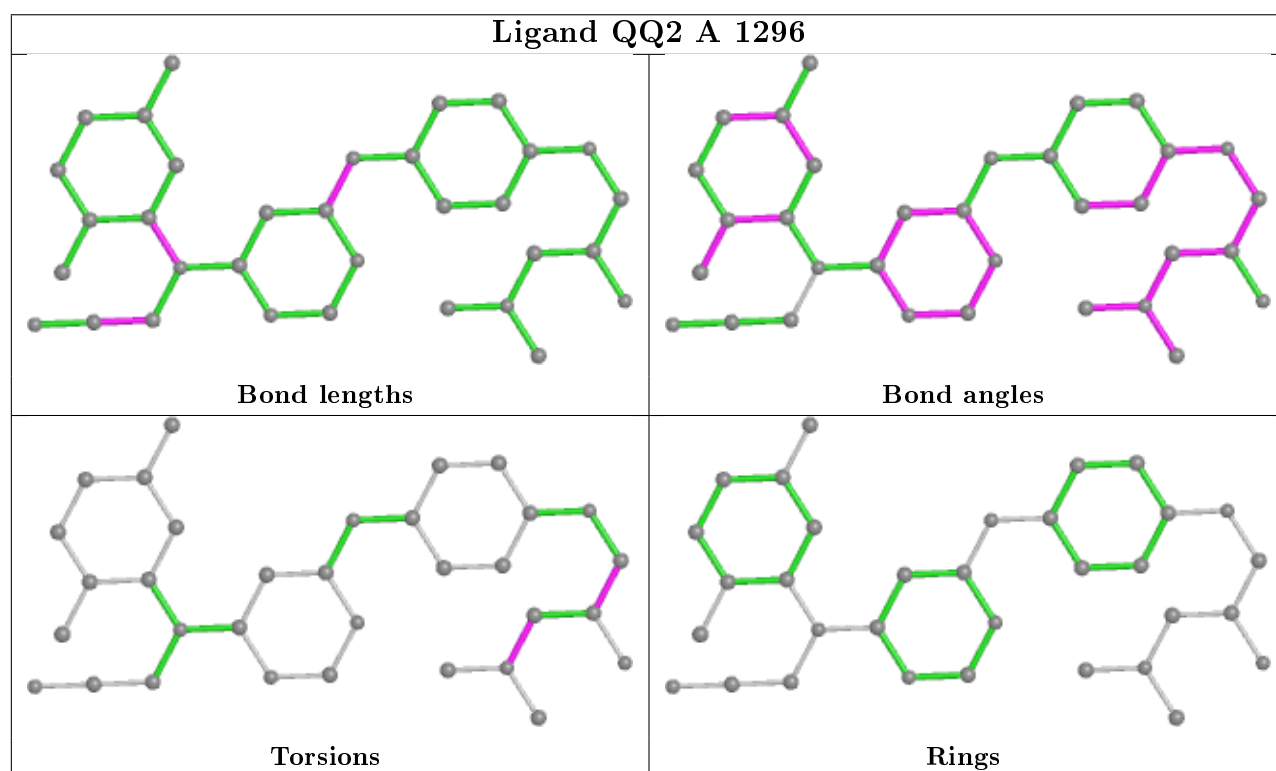
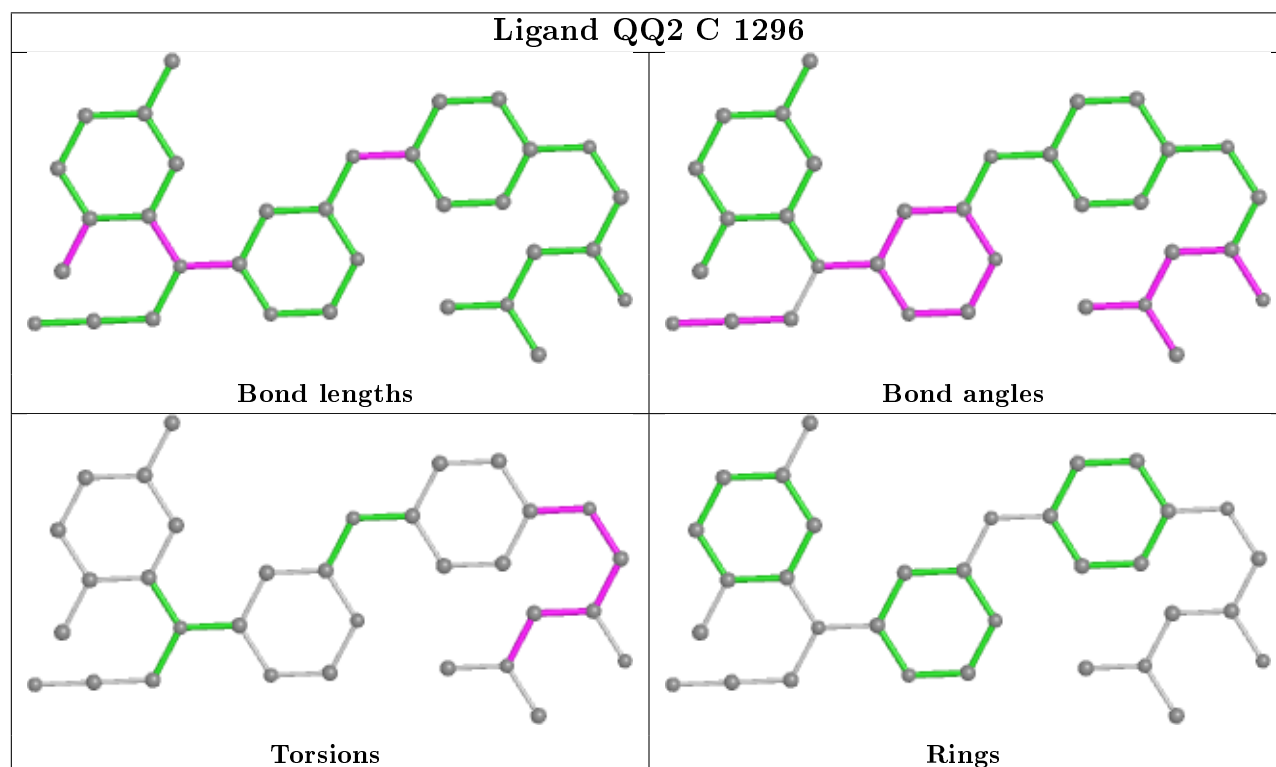
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1433	SGM	1	0
3	C	1296	QQ2	4	0
3	A	1296	QQ2	4	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.42	12 (4%) 37 44	26, 35, 46, 59	0
1	C	295/302 (97%)	1.10	54 (18%) 1 1	24, 35, 45, 58	0
2	B	257/260 (98%)	0.25	8 (3%) 49 56	29, 35, 44, 52	0
2	D	255/260 (98%)	1.00	52 (20%) 1 1	31, 36, 43, 48	0
All	All	1099/1124 (97%)	0.70	126 (11%) 4 7	24, 35, 45, 59	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	367	VAL	10.5
1	C	14	THR	9.4
1	C	234	PRO	7.6
2	D	368	THR	7.5
1	C	15	TYR	7.5
1	C	225	VAL	7.3
2	D	430	LEU	7.1
2	D	391	LEU	6.8
1	C	13	GLY	6.8
1	C	235	ASP	6.8
2	D	372	TRP	6.7
1	C	226	VAL	6.2
1	C	236	TYR	6.0
2	D	423	LEU	6.0
1	C	231	THR	5.8
1	C	287	GLN	5.4
2	D	364	LEU	5.4
2	D	395	HIS	5.4
2	D	428	GLU	5.3
1	C	239	SER	5.2
1	A	13	GLY	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	240	PHE	4.9
2	D	390	CYS	4.8
2	D	399	LEU	4.8
2	D	401	ALA	4.8
2	D	416	SER	4.7
1	A	73	GLU	4.7
1	C	257	GLU	4.7
2	D	421	VAL	4.6
1	C	238	PRO	4.5
1	C	233	MET	4.4
2	D	432	LEU	4.4
2	D	424	LEU	4.3
1	C	101	LEU	4.3
2	D	326	ASN	4.2
1	C	213	PHE	4.2
2	D	426	PRO	4.1
1	A	14	THR	4.1
2	D	366	THR	4.1
1	C	249	SER	4.0
1	C	258	ASP	4.0
1	C	175	LEU	4.0
1	C	209	ILE	4.0
1	C	284	PRO	4.0
1	C	232	SER	4.0
1	C	223	ASP	3.9
2	D	382	TYR	3.9
1	C	288	ASP	3.9
1	C	217	ARG	3.8
1	C	256	ASP	3.8
2	B	284	ASP	3.8
2	B	323	GLN	3.8
1	C	173	ILE	3.8
2	D	323	GLN	3.8
1	A	295	HIS	3.7
1	C	289	VAL	3.6
2	B	324	PRO	3.4
1	C	255	LEU	3.4
1	A	0	SER	3.4
1	A	162	GLU	3.4
2	D	415	ASN	3.4
1	C	237	LYS	3.4
1	C	247	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	327	CYS	3.3
2	D	392	MET	3.2
2	D	429	THR	3.2
1	C	252	VAL	3.2
2	D	375	SER	3.1
2	D	378	ARG	3.1
1	C	243	TRP	3.0
1	A	71	HIS	3.0
2	D	397	THR	3.0
1	C	36	ARG	3.0
2	D	350	TYR	2.9
1	C	286	PHE	2.9
2	B	432	LEU	2.9
2	D	402	PRO	2.9
1	C	290	THR	2.9
1	C	250	LYS	2.9
2	D	369	GLY	2.9
2	D	417	LYS	2.9
2	B	283	ASP	2.8
1	A	72	THR	2.8
2	D	377	ILE	2.8
1	C	241	PRO	2.8
1	A	15	TYR	2.7
2	D	419	HIS	2.7
1	C	246	GLN	2.7
2	D	365	TYR	2.7
1	A	95	ALA	2.7
2	D	283	ASP	2.6
2	D	333	ALA	2.6
1	C	285	PHE	2.6
2	D	387	LEU	2.6
1	C	102	PRO	2.6
2	B	280	TYR	2.6
1	C	245	ARG	2.6
1	A	96	LEU	2.6
2	D	411	GLU	2.6
1	C	224	GLU	2.5
1	C	221	THR	2.5
1	C	227	TRP	2.5
1	C	222	PRO	2.4
2	D	284	ASP	2.4
2	D	384	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	176	PRO	2.4
2	D	360	PHE	2.4
2	D	418	TYR	2.3
2	D	334	MET	2.3
1	C	229	GLY	2.3
1	C	205	GLY	2.2
2	D	388	LYS	2.2
2	D	398	TYR	2.2
2	B	285	THR	2.2
2	D	409	ILE	2.2
2	D	324	PRO	2.2
2	D	371	SER	2.2
1	C	74	ASN	2.2
2	D	346	PRO	2.2
1	C	162	GLU	2.1
1	C	244	ALA	2.1
2	D	385	GLU	2.1
1	A	36	ARG	2.1
2	D	422	SER	2.1
1	C	254	PRO	2.0
1	C	187	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.97	0.11	31,33,36,36	0
1	TPO	A	160	11/12	0.99	0.13	29,32,34,34	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

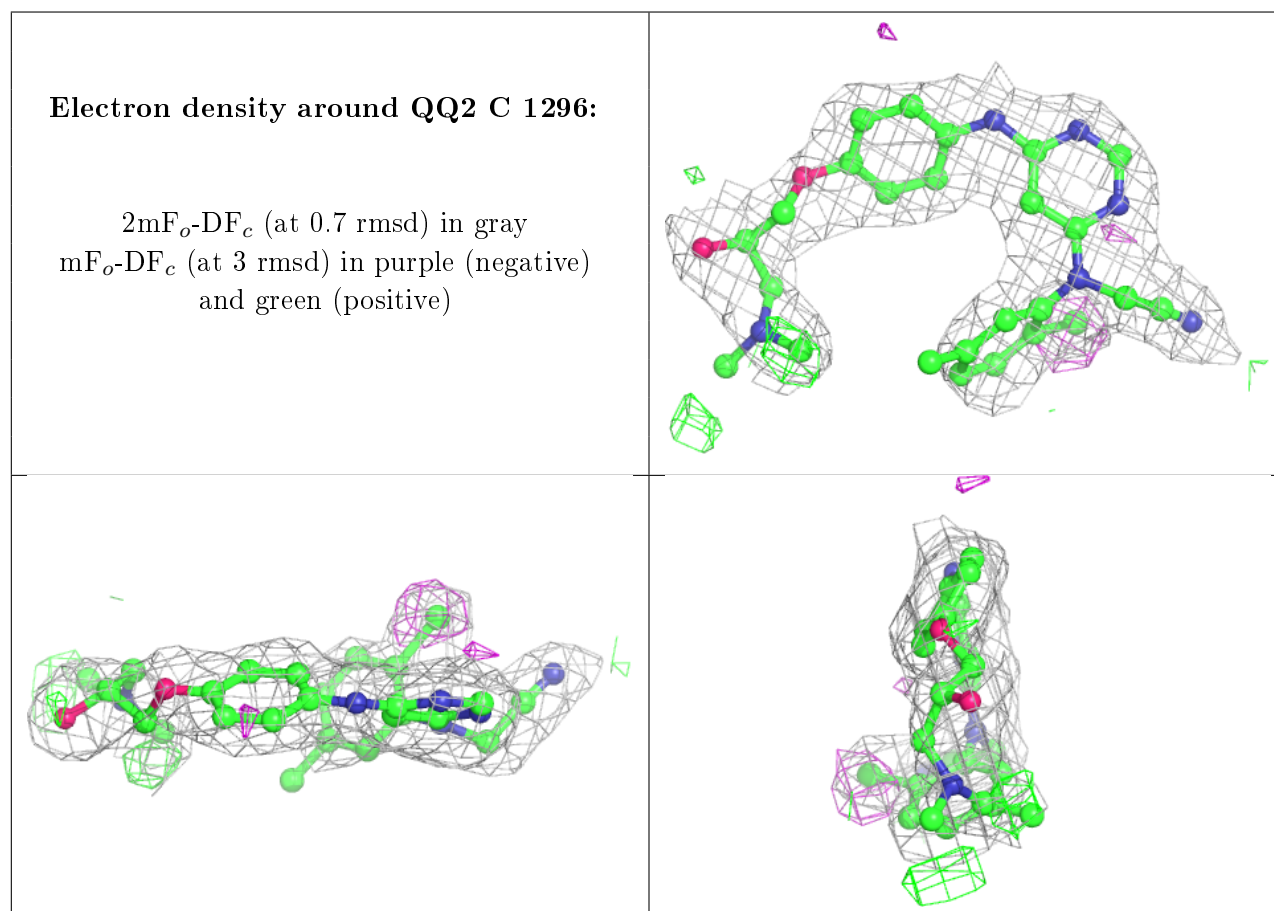
6.4 Ligands [i](#)

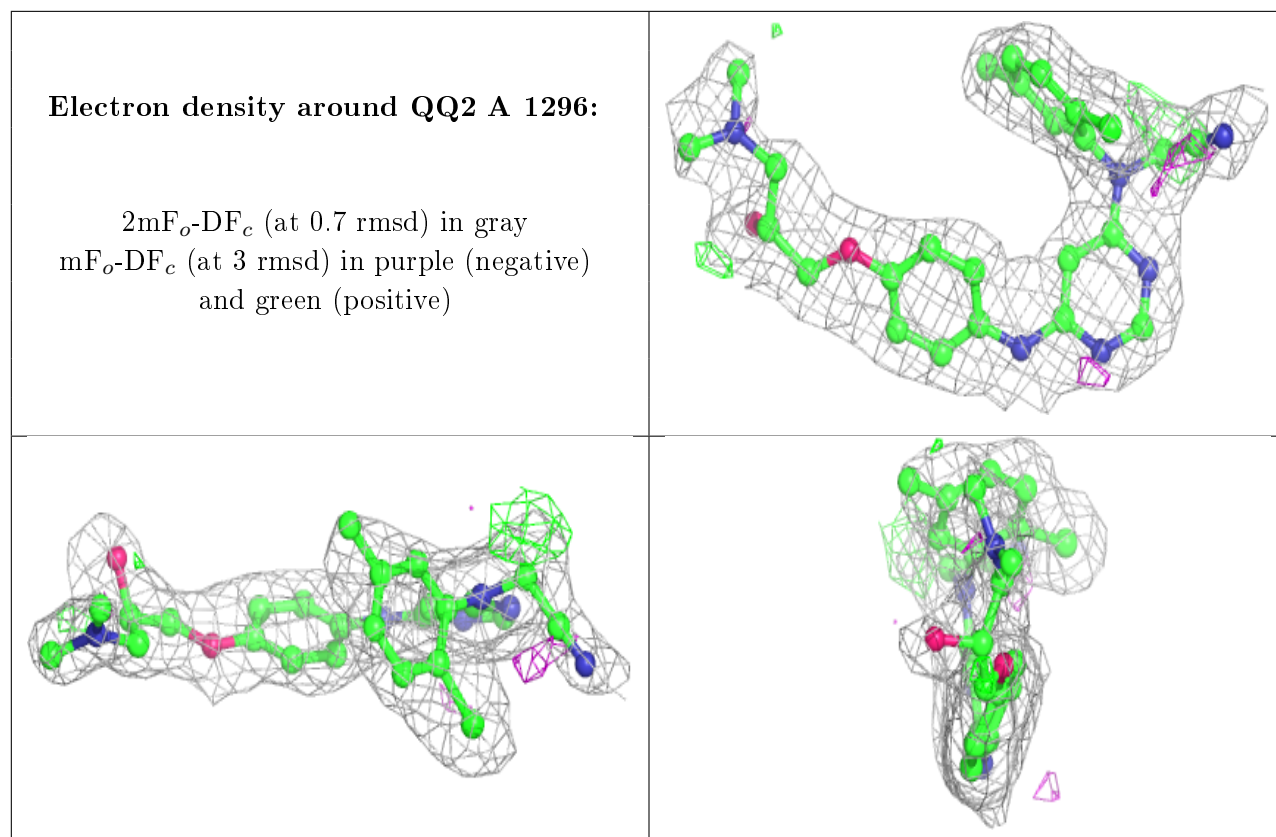
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	QQ2	C	1296	33/33	0.85	0.19	40,44,54,56	0
3	QQ2	A	1296	33/33	0.90	0.16	35,45,54,56	0
4	SGM	D	1433	6/6	0.92	0.14	54,55,55,56	0
5	MG	B	1434	1/1	0.94	0.08	31,31,31,31	0
4	SGM	B	1433	6/6	0.95	0.10	42,45,48,50	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.