



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:55 AM UTC

PDB ID : 4CFM / pdb_00004cfm
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 : 2013-11-18
Resolution : 2.85 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 Phenix2.0
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

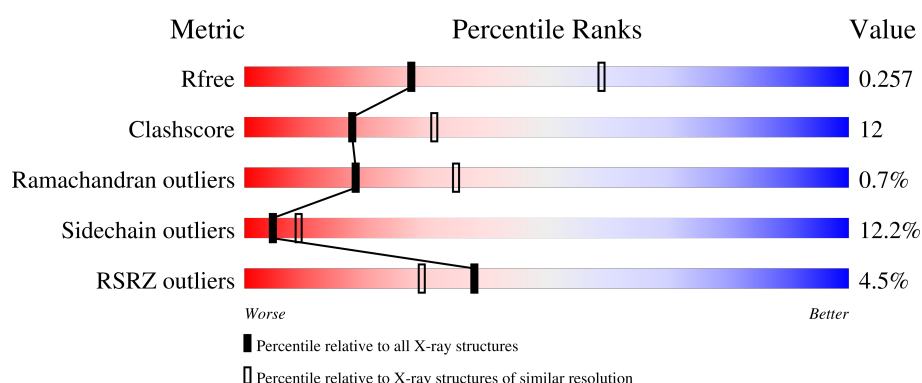
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	3% 63% 29% 5% ..
1	C	303	9% 60% 22% 5% • 12%
2	B	258	2% 69% 24% 7%
2	D	258	3% 71% 25% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8829 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	297	Total	C	N	O	P	S	0	5	0
			2425	1573	411	432	1	8			
1	C	267	Total	C	N	O	P	S	0	5	0
			2178	1410	372	388	1	7			

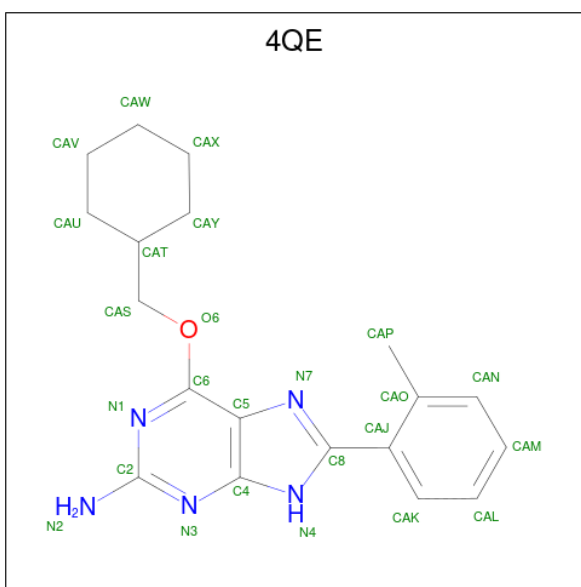
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	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	LEU	-	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	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is 6-(cyclohexylmethoxy)-8-(2-methylphenyl)-9H-purin-2-amine (CCD ID: 4QE) (formula: C₁₉H₂₃N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	19	5	1		
3	C	1	Total	C	N	O	0	0
			25	19	5	1		

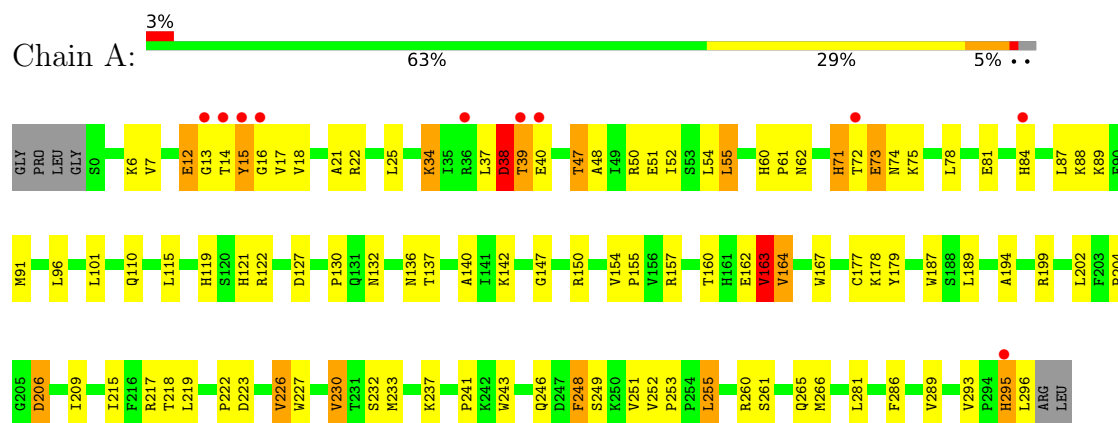
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	C	5	Total	O	0	0
			5	5		

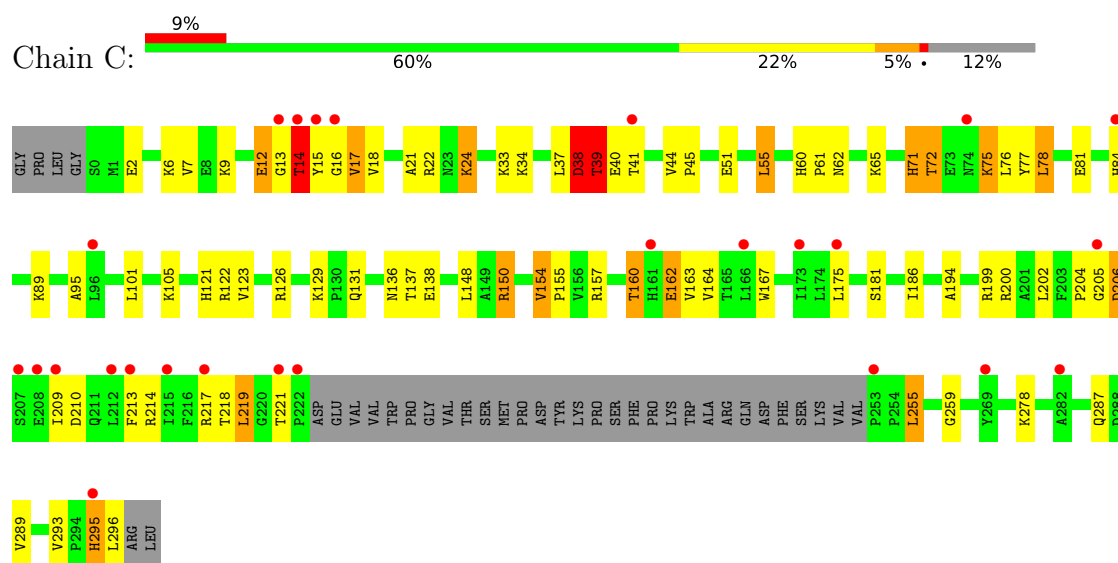
3 Residue-property plots

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.

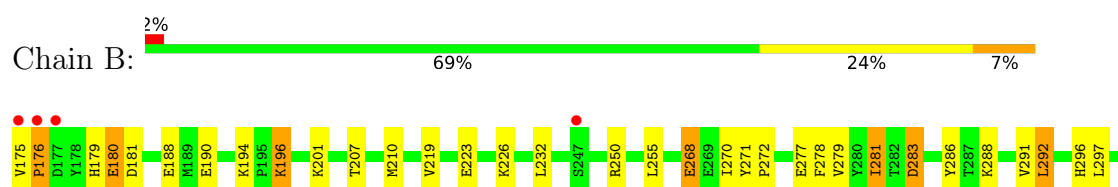
• Molecule 1: CYCLIN-DEPENDENT KINASE 2

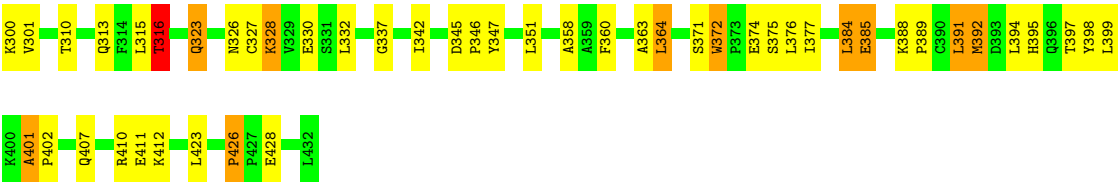


• Molecule 1: CYCLIN-DEPENDENT KINASE 2

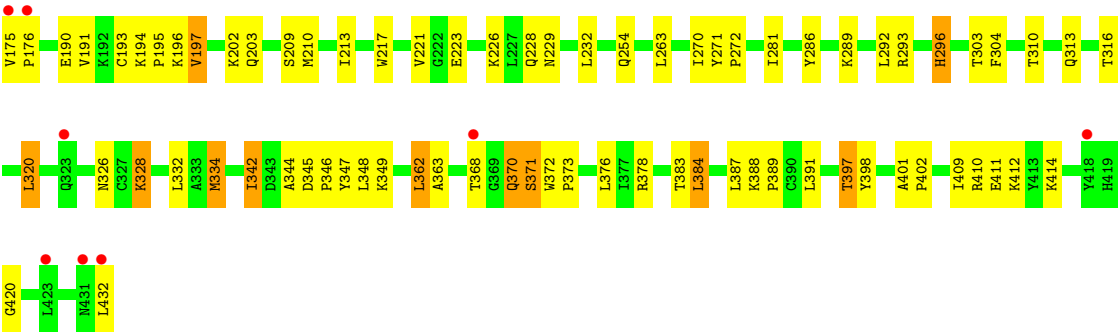


• Molecule 2: CYCLIN-A2





• 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	74.11Å 135.44Å 149.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.34 – 2.85 22.34 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.0 (22.34-2.85) 93.9 (22.34-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.84Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.217 , 0.258 0.216 , 0.257	Depositor DCC
R_{free} test set	1671 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8829	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4QE, 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	1.10	2/2477 (0.1%)	1.20	5/3361 (0.1%)
1	C	0.89	1/2218 (0.0%)	1.12	3/3003 (0.1%)
2	B	1.11	3/2133 (0.1%)	1.25	11/2897 (0.4%)
2	D	0.93	0/2133	1.16	7/2897 (0.2%)
All	All	1.02	6/8961 (0.1%)	1.18	26/12158 (0.2%)

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	2
1	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ASP	CA-C	6.59	1.61	1.52
2	B	401	ALA	C-O	-6.36	1.18	1.24
1	A	187	TRP	C-O	-5.49	1.17	1.24
1	C	76	LEU	C-O	-5.39	1.17	1.24
2	B	219	VAL	C-O	-5.36	1.17	1.24
2	B	385	GLU	C-O	-5.06	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	271	TYR	CA-C-N	-7.29	114.41	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	271	TYR	C-N-CA	-7.29	114.41	119.66
2	D	271	TYR	CA-C-N	-7.14	114.52	119.66
2	D	271	TYR	C-N-CA	-7.14	114.52	119.66
2	B	272	PRO	O-C-N	6.30	124.11	121.15
1	C	12	GLU	N-CA-C	6.29	118.65	109.15
2	D	197	VAL	CB-CA-C	-6.12	104.13	111.97
2	B	268	GLU	N-CA-C	5.97	120.70	113.41
2	B	316	THR	N-CA-CB	-5.97	101.11	110.06
2	B	426	PRO	O-C-N	5.96	124.05	121.31
1	A	253	PRO	N-CA-C	5.82	117.80	110.70
1	C	38	ASP	N-CA-C	5.79	123.13	110.80
1	A	17	VAL	CB-CA-C	-5.70	101.94	111.29
2	D	272	PRO	O-C-N	5.64	123.80	121.15
1	A	163	VAL	N-CA-C	5.64	115.79	108.35
2	D	203	GLN	CA-C-N	-5.54	114.06	120.04
2	D	203	GLN	C-N-CA	-5.54	114.06	120.04
2	B	196	LYS	CB-CA-C	5.54	118.87	109.84
1	A	38	ASP	N-CA-C	5.42	122.34	110.80
2	B	337	GLY	N-CA-C	-5.37	106.27	112.50
2	D	191	VAL	CB-CA-C	-5.27	104.94	112.22
2	B	372	TRP	CA-C-N	5.25	125.16	119.85
2	B	372	TRP	C-N-CA	5.25	125.16	119.85
1	A	248	PHE	N-CA-C	5.18	117.67	111.71
2	B	175	VAL	CB-CA-C	5.15	121.19	111.40
1	C	71	HIS	N-CA-C	5.03	117.81	109.46

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLU	Peptide
1	A	38	ASP	Peptide
1	C	12	GLU	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	2425	0	2457	79	0
1	C	2178	0	2220	64	0
2	B	2083	0	2107	48	0
2	D	2083	0	2107	45	0
3	A	25	0	23	4	0
3	C	25	0	23	5	0
4	A	5	0	0	0	0
4	C	5	0	0	1	0
All	All	8829	0	8937	218	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 12.

All (218) 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:C:84[B]:HIS:CD2	1:C:296:LEU:CD1	2.09	1.36
1:C:84[B]:HIS:HD2	1:C:296:LEU:HD13	0.99	1.14
1:C:84[B]:HIS:CD2	1:C:296:LEU:HD13	1.75	1.09
1:C:84[B]:HIS:CD2	1:C:296:LEU:HD12	1.81	1.09
1:A:84[B]:HIS:HD2	1:A:296:LEU:HD13	1.19	1.04
2:B:392:MET:HE2	2:B:392:MET:HA	1.44	0.99
1:C:84[B]:HIS:HD2	1:C:296:LEU:CD1	1.63	0.96
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.83	0.96
1:A:87:LEU:HG	1:A:91:MET:HE2	1.50	0.93
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.41	0.88
1:A:60:HIS:CD2	1:A:62:ASN:H	1.95	0.84
1:C:38:ASP:O	1:C:39:THR:HB	1.78	0.83
1:A:84[B]:HIS:HD2	1:A:296:LEU:CD1	1.91	0.83
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.66	0.83
1:A:71:HIS:CD2	2:B:296:HIS:CE1	2.67	0.82
1:A:81:GLU:O	3:A:1297:4QE:N2	2.13	0.81
1:A:15[A]:TYR:HD1	1:A:15[A]:TYR:N	1.77	0.80
1:C:95:ALA:O	1:C:199:ARG:NH1	2.14	0.80
1:A:60:HIS:HD2	1:A:62:ASN:H	1.29	0.80
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.64	0.79
1:A:71:HIS:HD2	2:B:296:HIS:NE2	1.80	0.78
1:A:84[B]:HIS:CD2	1:A:296:LEU:HD13	2.12	0.77
1:A:39:THR:HA	2:B:292:LEU:HD23	1.67	0.76
1:A:154:VAL:O	2:B:316:THR:CG2	2.34	0.75
1:C:84[A]:HIS:CD2	1:C:136:ASN:HA	2.21	0.75
2:D:347:TYR:HH	2:D:397:THR:HG1	1.30	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:O	2:B:316:THR:HG22	1.87	0.73
1:C:81:GLU:O	3:C:1297:4QE:N2	2.22	0.73
1:A:249:SER:HA	1:A:260:ARG:HD3	1.71	0.73
1:C:60:HIS:CD2	1:C:62:ASN:H	2.06	0.73
1:A:15[A]:TYR:N	1:A:15[A]:TYR:CD1	2.50	0.71
1:C:154:VAL:O	2:D:316:THR:HG23	1.91	0.70
1:A:121:HIS:O	1:A:122:ARG:HG3	1.93	0.69
3:C:1297:4QE:H9	4:C:2003:HOH:O	1.92	0.68
1:A:51:GLU:O	1:A:55:LEU:HB2	1.93	0.68
1:C:126:ARG:HD2	1:C:163:VAL:HG11	1.74	0.68
1:C:155:PRO:HG3	2:D:320:LEU:HD21	1.75	0.68
1:A:13[A]:GLY:HA2	3:A:1297:4QE:H3	1.76	0.67
1:A:177:CYS:HB2	1:A:233:MET:HE2	1.75	0.67
1:C:51:GLU:O	1:C:55:LEU:HB2	1.94	0.67
1:A:16[B]:GLY:HA3	1:A:34:LYS:O	1.95	0.67
1:C:84[A]:HIS:HD2	1:C:136:ASN:HA	1.59	0.66
2:B:347:TYR:OH	2:B:394:LEU:HA	1.95	0.66
2:B:392:MET:HE2	2:B:392:MET:CA	2.24	0.65
1:C:121:HIS:O	1:C:122:ARG:HG3	1.96	0.65
1:A:71:HIS:HD2	2:B:296:HIS:CE1	2.07	0.65
1:A:25:LEU:HD11	2:D:293:ARG:HB3	1.79	0.65
1:C:14[A]:THR:HB	1:C:15[A]:TYR:HD1	1.62	0.65
1:A:38:ASP:O	1:A:39:THR:HB	1.98	0.63
1:A:177:CYS:HB2	1:A:233:MET:CE	2.28	0.63
1:C:213:PHE:HB3	1:C:217:ARG:CZ	2.29	0.62
1:C:84[B]:HIS:NE2	1:C:296:LEU:HD12	2.12	0.62
1:A:194:ALA:CB	1:A:202:LEU:HD22	2.29	0.62
2:B:278:PHE:HA	2:B:281:ILE:HD11	1.80	0.61
1:C:13[A]:GLY:HA2	3:C:1297:4QE:H3	1.82	0.61
1:A:84[B]:HIS:CD2	1:A:296:LEU:CD1	2.78	0.61
2:B:190:GLU:HG3	2:B:351:LEU:HD22	1.83	0.61
1:A:227:TRP:O	1:A:230:VAL:HG22	2.00	0.60
1:A:295:HIS:O	1:A:295:HIS:CG	2.51	0.60
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.84	0.59
1:A:252:VAL:CG1	1:A:255:LEU:HD22	2.31	0.59
1:A:121:HIS:C	1:A:122:ARG:HG3	2.27	0.59
1:A:261:SER:O	1:A:265:GLN:HG3	2.03	0.58
2:B:268:GLU:HG3	2:B:268:GLU:O	2.04	0.57
2:D:254:GLN:HG2	2:D:286:TYR:HE2	1.68	0.57
1:A:252:VAL:HG11	1:A:255:LEU:HD22	1.87	0.57
2:D:370:GLN:H	2:D:370:GLN:HE21	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14[A]:THR:C	1:A:15[A]:TYR:HD1	2.13	0.56
2:D:310:THR:HG23	2:D:313:GLN:HE21	1.70	0.56
1:C:13[A]:GLY:HA2	3:C:1297:4QE:CAV	2.35	0.56
1:C:121:HIS:C	1:C:122:ARG:HG3	2.31	0.56
1:C:295:HIS:O	1:C:295:HIS:CD2	2.59	0.55
2:B:392:MET:HA	2:B:392:MET:CE	2.28	0.55
1:C:84[A]:HIS:CD2	1:C:84[A]:HIS:N	2.74	0.55
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.88	0.55
2:B:310:THR:HG23	2:B:313:GLN:HE21	1.72	0.55
1:A:127:ASP:O	1:A:132:ASN:ND2	2.39	0.54
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.23	0.54
1:A:178:LYS:HE2	1:A:179:TYR:CZ	2.43	0.54
1:A:71:HIS:CD2	2:B:296:HIS:HE2	2.26	0.54
1:C:34:LYS:HG3	1:C:77:TYR:CE1	2.43	0.54
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.90	0.54
1:C:39:THR:CG2	1:C:40:GLU:N	2.71	0.54
2:D:342:ILE:HD11	2:D:409:ILE:CD1	2.38	0.54
2:D:370:GLN:H	2:D:370:GLN:NE2	2.06	0.53
1:C:84[A]:HIS:CD2	1:C:84[A]:HIS:H	2.26	0.53
1:A:71:HIS:HD2	2:B:296:HIS:HE2	1.54	0.53
1:C:15[A]:TYR:CE2	1:C:33:LYS:HE2	2.44	0.52
1:C:71:HIS:CD2	2:D:296:HIS:HE1	2.23	0.52
1:C:60:HIS:HD2	1:C:62:ASN:H	1.51	0.52
1:C:2:GLU:O	1:C:24:LYS:NZ	2.42	0.52
2:D:346:PRO:O	2:D:349:LYS:HG2	2.09	0.52
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.93	0.51
2:B:327:CYS:HA	2:B:330:GLU:HG3	1.93	0.51
1:C:18:VAL:HG21	3:C:1297:4QE:H1	1.91	0.51
2:D:373:PRO:HD2	2:D:376:LEU:HD12	1.93	0.51
1:A:218:THR:HG22	1:A:219:LEU:HD23	1.92	0.51
2:B:297:LEU:O	2:B:301:VAL:HG23	2.11	0.51
1:C:14[A]:THR:HB	1:C:15[A]:TYR:CD1	2.44	0.50
1:C:16[B]:GLY:HA3	1:C:34:LYS:O	2.12	0.50
1:C:218:THR:HG22	1:C:219:LEU:HD23	1.94	0.50
1:C:72:THR:HB	1:C:75:LYS:H	1.76	0.50
2:D:378:ARG:HB2	2:D:378:ARG:NH1	2.28	0.49
2:D:346:PRO:HB2	2:D:349:LYS:HE2	1.93	0.49
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.95	0.48
1:A:39:THR:CG2	1:A:40:GLU:N	2.76	0.48
2:D:362:LEU:HD21	2:D:398:TYR:HD2	1.78	0.48
1:A:206:ASP:OD1	1:A:206:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:384:LEU:HD11	2:D:432:LEU:HD22	1.94	0.48
1:A:223:ASP:H	1:A:226:VAL:CG1	2.26	0.48
2:B:358:ALA:HB1	2:B:391:LEU:HD13	1.96	0.48
1:C:78:LEU:HD23	1:C:78:LEU:N	2.28	0.48
1:C:162:GLU:N	1:C:162:GLU:OE1	2.47	0.48
1:A:14[A]:THR:C	1:A:15[A]:TYR:CD1	2.90	0.47
1:C:126:ARG:HB3	1:C:163:VAL:CG1	2.44	0.47
1:C:150:ARG:NH2	1:C:160:TPO:O2P	2.47	0.47
2:B:223:GLU:CD	2:B:412:LYS:HG3	2.39	0.47
1:C:39:THR:HG23	1:C:40:GLU:H	1.78	0.47
1:A:7:VAL:HG23	1:A:21:ALA:HA	1.96	0.47
1:C:194:ALA:HB1	1:C:202:LEU:HD13	1.96	0.47
1:A:13[B]:GLY:C	1:A:14[B]:THR:HG23	2.40	0.47
1:A:255:LEU:O	1:A:260:ARG:NH1	2.48	0.47
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.96	0.47
1:A:115:LEU:HD11	1:A:119:HIS:CE1	2.50	0.47
1:A:13[B]:GLY:C	1:A:14[B]:THR:CG2	2.88	0.47
1:C:39:THR:HG22	1:C:40:GLU:OE2	2.15	0.47
2:D:223:GLU:OE1	2:D:412:LYS:HE3	2.13	0.47
1:A:137:THR:HG22	1:A:296:LEU:HD12	1.96	0.46
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.96	0.46
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.98	0.46
2:B:326:ASN:OD1	2:B:328:LYS:HB3	2.16	0.46
2:B:384:LEU:HD12	2:B:384:LEU:HA	1.51	0.46
1:C:105:LYS:HG2	1:C:289:VAL:HG23	1.98	0.46
2:D:217:TRP:O	2:D:221:VAL:HG23	2.15	0.46
1:A:48:ALA:O	1:A:52:ILE:HG13	2.16	0.46
1:A:47:THR:HG22	1:A:147:GLY:O	2.16	0.45
1:C:213:PHE:HB3	1:C:217:ARG:NH2	2.30	0.45
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.97	0.45
1:A:223:ASP:H	1:A:226:VAL:HG12	1.82	0.45
1:A:189:LEU:HB3	1:A:266:MET:HE1	1.98	0.45
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.81	0.45
1:A:50:ARG:O	1:A:54:LEU:HG	2.16	0.45
2:B:407:GLN:O	2:B:411:GLU:HG2	2.16	0.45
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.98	0.45
2:B:279:VAL:HG21	2:B:288:LYS:HA	1.98	0.45
1:C:121:HIS:O	1:C:123:VAL:HG23	2.16	0.45
2:D:345:ASP:HA	2:D:346:PRO:HA	1.75	0.45
1:A:13[A]:GLY:HA2	3:A:1297:4QE:CAV	2.45	0.45
2:B:392:MET:CA	2:B:392:MET:CE	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.51	0.45
1:A:163:VAL:C	1:A:164:VAL:HG23	2.42	0.45
2:D:401:ALA:N	2:D:402:PRO:HD2	2.32	0.45
2:B:346:PRO:HD2	2:B:347:TYR:CD2	2.51	0.44
1:C:157:ARG:NH2	2:D:228:GLN:HG3	2.32	0.44
1:C:206:ASP:OD1	1:C:206:ASP:N	2.50	0.44
1:A:61:PRO:O	1:A:142:LYS:HE2	2.18	0.44
1:A:39:THR:HG22	1:A:40:GLU:N	2.31	0.44
1:C:136:ASN:HD21	1:C:138:GLU:HB2	1.83	0.44
2:D:229:ASN:HD22	2:D:334:MET:HE2	1.83	0.44
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.53	0.43
1:C:39:THR:HG22	1:C:40:GLU:CD	2.42	0.43
2:D:326:ASN:OD1	2:D:328:LYS:HB2	2.18	0.43
2:D:371:SER:O	2:D:372:TRP:C	2.60	0.43
1:A:209:ILE:HD12	1:A:209:ILE:HA	1.84	0.43
1:C:39:THR:HG21	2:D:289:LYS:NZ	2.34	0.43
2:B:194:LYS:HD3	2:B:351:LEU:HD23	2.00	0.43
2:B:374:GLU:HA	2:B:377:ILE:HD12	2.00	0.43
1:A:136:ASN:ND2	1:A:140:ALA:HB3	2.34	0.43
2:B:207:THR:OG1	2:B:210:MET:HG3	2.19	0.43
1:A:72:THR:HG22	1:A:73:GLU:H	1.83	0.43
1:A:189:LEU:HA	1:A:189:LEU:HD23	1.73	0.43
2:B:345:ASP:HA	2:B:346:PRO:HA	1.84	0.43
2:B:376:LEU:HD23	2:B:376:LEU:HA	1.77	0.43
1:A:249:SER:CA	1:A:260:ARG:HD3	2.47	0.43
2:B:315:LEU:HD23	2:B:315:LEU:HA	1.84	0.43
2:B:395:HIS:CE1	2:B:399:LEU:HD11	2.54	0.43
2:D:344:ALA:HB1	2:D:348:LEU:HD22	2.01	0.43
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.54	0.43
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.54	0.43
1:A:222:PRO:HA	1:A:226:VAL:HG11	2.00	0.42
1:C:131:GLN:H	1:C:131:GLN:CD	2.27	0.42
2:D:210:MET:O	2:D:213:ILE:HB	2.19	0.42
1:C:9:LYS:HE2	1:C:17:VAL:HG11	2.01	0.42
2:B:371:SER:O	2:B:372:TRP:C	2.62	0.42
2:D:410:ARG:O	2:D:414:LYS:HG3	2.20	0.42
2:D:303:THR:O	2:D:304:PHE:HB2	2.19	0.42
1:A:39:THR:CG2	1:A:40:GLU:H	2.32	0.42
2:B:180:GLU:OE1	2:B:180:GLU:HA	2.18	0.42
1:C:205:GLY:HA2	1:C:210:ASP:OD1	2.20	0.41
2:B:360:PHE:CZ	2:B:364:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:VAL:HA	2:D:176:PRO:HD3	1.89	0.41
2:D:342:ILE:HD11	2:D:409:ILE:HD11	2.02	0.41
2:B:255:LEU:HB2	2:B:286:TYR:CZ	2.55	0.41
1:C:295:HIS:O	1:C:295:HIS:CG	2.74	0.41
1:A:241:PRO:HG2	1:A:243:TRP:CH2	2.55	0.41
1:A:286:PHE:O	1:A:289:VAL:HG12	2.20	0.41
1:C:7:VAL:HG23	1:C:21:ALA:HA	2.03	0.41
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.56	0.41
2:D:223:GLU:CD	2:D:412:LYS:HG3	2.45	0.41
2:D:194:LYS:HA	2:D:195:PRO:HD3	1.95	0.41
1:A:87:LEU:HA	1:A:87:LEU:HD12	1.85	0.41
2:D:376:LEU:HD23	2:D:376:LEU:HA	1.94	0.41
1:A:18:VAL:HG21	3:A:1297:4QE:H1	2.03	0.41
2:B:407:GLN:OE1	2:B:410:ARG:HD3	2.21	0.41
2:D:190:GLU:O	2:D:194:LYS:HB2	2.21	0.41
2:D:263:LEU:HD23	2:D:263:LEU:HA	1.96	0.41
2:B:385:GLU:HA	2:B:385:GLU:OE1	2.21	0.41
1:C:71:HIS:CE1	2:D:304:PHE:HE2	2.39	0.41
2:D:372:TRP:CZ3	2:D:376:LEU:HD13	2.55	0.41
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.02	0.40
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.56	0.40
2:D:310:THR:HG23	2:D:313:GLN:NE2	2.34	0.40
1:C:202:LEU:HD12	1:C:202:LEU:HA	1.83	0.40
2:D:383:THR:O	2:D:387:LEU:HD12	2.22	0.40
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.36	0.40
1:A:227:TRP:HB3	1:A:230:VAL:HG22	2.03	0.40
2:B:323:GLN:HA	2:B:323:GLN:OE1	2.21	0.40
1:C:44:VAL:HA	1:C:45:PRO:HD2	1.93	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	299/303 (99%)	278 (93%)	19 (6%)	2 (1%)	18	35
1	C	267/303 (88%)	247 (92%)	15 (6%)	5 (2%)	6	14
2	B	256/258 (99%)	249 (97%)	5 (2%)	2 (1%)	16	31
2	D	256/258 (99%)	248 (97%)	8 (3%)	0	100	100
All	All	1078/1122 (96%)	1022 (95%)	47 (4%)	9 (1%)	18	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	283	ASP
1	A	162	GLU
1	A	164	VAL
1	C	164	VAL
1	C	39	THR
2	B	176	PRO
1	C	14[A]	THR
1	C	14[B]	THR
1	C	162	GLU

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	264/265 (100%)	230 (87%)	34 (13%)	4	7
1	C	236/265 (89%)	200 (85%)	36 (15%)	3	5
2	B	232/232 (100%)	206 (89%)	26 (11%)	6	11
2	D	232/232 (100%)	209 (90%)	23 (10%)	7	16
All	All	964/994 (97%)	845 (88%)	119 (12%)	5	8

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	12	GLU

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Mol	Chain	Res	Type
1	A	15[A]	TYR
1	A	15[B]	TYR
1	A	22	ARG
1	A	34	LYS
1	A	37	LEU
1	A	39	THR
1	A	47	THR
1	A	55	LEU
1	A	71	HIS
1	A	73	GLU
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	89	LYS
1	A	96	LEU
1	A	101	LEU
1	A	150	ARG
1	A	157	ARG
1	A	163	VAL
1	A	199	ARG
1	A	206	ASP
1	A	215	ILE
1	A	226	VAL
1	A	230	VAL
1	A	232	SER
1	A	237	LYS
1	A	246	GLN
1	A	248	PHE
1	A	255	LEU
1	A	281	LEU
1	A	293	VAL
1	A	295	HIS
2	B	180	GLU
2	B	181	ASP
2	B	188	GLU
2	B	196	LYS
2	B	201	LYS
2	B	226	LYS
2	B	232	LEU
2	B	270	ILE
2	B	277	GLU
2	B	281	ILE

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Mol	Chain	Res	Type
2	B	283	ASP
2	B	291	VAL
2	B	292	LEU
2	B	300	LYS
2	B	316	THR
2	B	323	GLN
2	B	328	LYS
2	B	342	ILE
2	B	364	LEU
2	B	375	SER
2	B	384	LEU
2	B	391	LEU
2	B	392	MET
2	B	397	THR
2	B	423	LEU
2	B	428	GLU
1	C	6	LYS
1	C	14[A]	THR
1	C	14[B]	THR
1	C	17	VAL
1	C	22	ARG
1	C	24	LYS
1	C	37	LEU
1	C	38	ASP
1	C	39	THR
1	C	41	THR
1	C	55	LEU
1	C	65	LYS
1	C	72	THR
1	C	75	LYS
1	C	78	LEU
1	C	89	LYS
1	C	101	LEU
1	C	129	LYS
1	C	137	THR
1	C	148	LEU
1	C	150	ARG
1	C	154	VAL
1	C	175	LEU
1	C	181	SER
1	C	186	ILE
1	C	200	ARG

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Mol	Chain	Res	Type
1	C	206	ASP
1	C	209	ILE
1	C	214	ARG
1	C	219	LEU
1	C	221	THR
1	C	255	LEU
1	C	278	LYS
1	C	287	GLN
1	C	293	VAL
1	C	295	HIS
2	D	193	CYS
2	D	196	LYS
2	D	197	VAL
2	D	202	LYS
2	D	209	SER
2	D	226	LYS
2	D	232	LEU
2	D	270	ILE
2	D	281	ILE
2	D	292	LEU
2	D	296	HIS
2	D	320	LEU
2	D	328	LYS
2	D	334	MET
2	D	342	ILE
2	D	362	LEU
2	D	368	THR
2	D	370	GLN
2	D	371	SER
2	D	384	LEU
2	D	391	LEU
2	D	397	THR
2	D	411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	265	GLN
2	B	179	HIS
2	B	254	GLN

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Mol	Chain	Res	Type
2	B	313	GLN
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	119	HIS
1	C	295	HIS
2	D	229	ASN
2	D	254	GLN
2	D	296	HIS
2	D	313	GLN
2	D	370	GLN
2	D	395	HIS
2	D	396	GLN
2	D	403	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	0.69	0	10,14,16	1.42	1 (10%)
1	TPO	A	160	1	8,10,11	1.07	0	10,14,16	1.84	2 (20%)

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	-	2/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	OG1-P-O1P	-4.10	94.73	109.33
1	A	160	TPO	O3P-P-O2P	2.24	116.22	107.80
1	C	160	TPO	OG1-P-O1P	-2.15	101.68	109.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	CB-OG1-P-O1P
1	C	160	TPO	O-C-CA-CB
1	A	160	TPO	CB-OG1-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	4QE	C	1297	-	28,28,28	2.35	7 (25%)	37,39,39	1.77	10 (27%)
3	4QE	A	1297	-	28,28,28	2.26	8 (28%)	37,39,39	1.99	10 (27%)

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	4QE	C	1297	-	-	2/9/17/17	0/4/4/4
3	4QE	A	1297	-	-	2/9/17/17	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1297	4QE	CAJ-C8	-7.40	1.34	1.47
3	A	1297	4QE	CAJ-C8	-6.63	1.35	1.47
3	A	1297	4QE	CAP-CAO	-5.75	1.40	1.51
3	C	1297	4QE	CAP-CAO	-5.38	1.40	1.51
3	C	1297	4QE	C4-N4	-4.26	1.32	1.37
3	A	1297	4QE	C4-N4	-4.06	1.32	1.37
3	C	1297	4QE	C5-C6	-3.70	1.34	1.41
3	C	1297	4QE	C5-C4	-3.07	1.34	1.39
3	C	1297	4QE	C5-N7	-3.07	1.34	1.39
3	A	1297	4QE	C5-N7	-2.97	1.34	1.39
3	A	1297	4QE	C5-C4	-2.85	1.34	1.39
3	A	1297	4QE	C5-C6	-2.82	1.36	1.41
3	A	1297	4QE	CAV-CAU	-2.31	1.47	1.53
3	A	1297	4QE	O6-C6	2.08	1.38	1.34
3	C	1297	4QE	O6-C6	2.02	1.37	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1297	4QE	C5-C4-N3	-6.36	120.31	126.55
3	C	1297	4QE	C5-C4-N3	-5.52	121.14	126.55
3	A	1297	4QE	C4-C5-C6	3.86	119.19	115.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297	4QE	C4-C5-C6	3.78	119.11	115.38
3	C	1297	4QE	N3-C2-N1	-3.19	120.60	125.48
3	A	1297	4QE	O6-C6-C5	3.03	120.73	116.73
3	A	1297	4QE	C4-C5-N7	-2.97	106.53	110.64
3	A	1297	4QE	N3-C2-N1	-2.95	120.97	125.48
3	A	1297	4QE	CAY-CAT-CAS	-2.69	104.26	111.42
3	C	1297	4QE	CAY-CAT-CAS	-2.63	104.39	111.42
3	C	1297	4QE	C2-N1-C6	2.49	119.42	115.96
3	C	1297	4QE	C5-C6-N1	-2.41	120.26	123.49
3	A	1297	4QE	C5-C6-N1	-2.41	120.27	123.49
3	A	1297	4QE	C2-N3-C4	2.39	120.27	114.59
3	A	1297	4QE	C2-N1-C6	2.18	118.99	115.96
3	C	1297	4QE	CAY-CAT-CAU	2.15	114.55	109.29
3	A	1297	4QE	CAN-CAO-CAJ	2.07	120.25	117.75
3	C	1297	4QE	C2-N3-C4	2.05	119.47	114.59
3	C	1297	4QE	N4-C4-N3	2.01	129.77	125.30
3	C	1297	4QE	C4-C5-N7	-2.00	107.87	110.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1297	4QE	N1-C6-O6-CAS
3	A	1297	4QE	C5-C6-O6-CAS
3	C	1297	4QE	N1-C6-O6-CAS
3	C	1297	4QE	C5-C6-O6-CAS

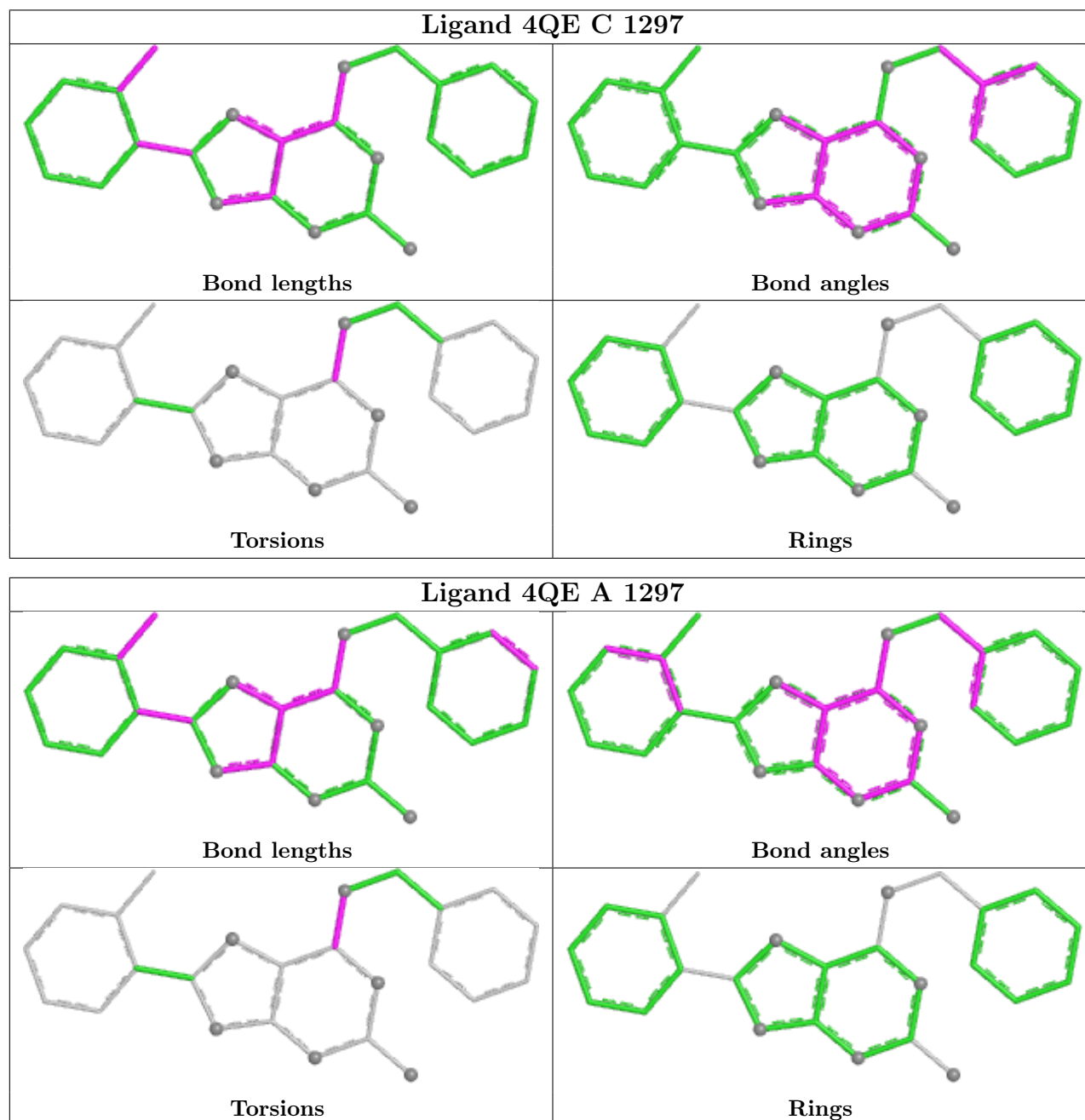
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	4QE	5	0
3	A	1297	4QE	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 [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/303 (97%)	-0.31	10 (3%) 48 38	22, 36, 60, 80	5 (1%)
1	C	266/303 (87%)	0.52	26 (9%) 13 10	30, 73, 120, 144	5 (1%)
2	B	258/258 (100%)	-0.40	4 (1%) 70 64	24, 39, 55, 63	0
2	D	258/258 (100%)	0.27	8 (3%) 51 43	39, 75, 134, 156	0
All	All	1078/1122 (96%)	0.01	48 (4%) 38 29	22, 50, 117, 156	10 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14[A]	THR	5.1
1	C	253	PRO	5.0
1	C	213	PHE	4.7
2	B	175	VAL	4.4
1	C	217	ARG	4.2
1	C	13[A]	GLY	4.1
1	C	15[A]	TYR	4.1
2	D	176	PRO	4.0
1	A	14[A]	THR	4.0
1	A	16[A]	GLY	3.9
1	C	209	ILE	3.8
1	C	96	LEU	3.7
1	A	13[A]	GLY	3.7
2	D	175	VAL	3.5
1	C	222	PRO	3.4
1	A	15[A]	TYR	3.4
1	A	36	ARG	3.3
1	C	84[A]	HIS	3.2
1	C	205	GLY	3.2
1	C	221	THR	3.1
2	D	431	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	166	LEU	3.0
1	C	282	ALA	2.8
1	C	212	LEU	2.8
1	C	269	TYR	2.7
1	C	41	THR	2.7
1	C	74	ASN	2.6
1	C	207	SER	2.5
1	A	40	GLU	2.5
2	B	176	PRO	2.5
1	A	84[A]	HIS	2.5
1	C	175	LEU	2.4
1	A	72	THR	2.3
1	A	295	HIS	2.3
1	A	39	THR	2.3
2	D	368	THR	2.3
1	C	208	GLU	2.2
1	C	161	HIS	2.2
1	C	295	HIS	2.2
1	C	173	ILE	2.1
2	D	323	GLN	2.1
1	C	16[A]	GLY	2.1
1	C	215	ILE	2.1
2	B	177	ASP	2.1
2	D	418	TYR	2.1
2	B	247	SER	2.0
2	D	423	LEU	2.0
2	D	432	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.90	0.11	72,78,82,84	0
1	TPO	A	160	11/12	0.98	0.07	31,32,34,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

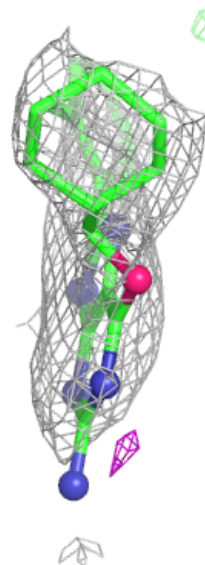
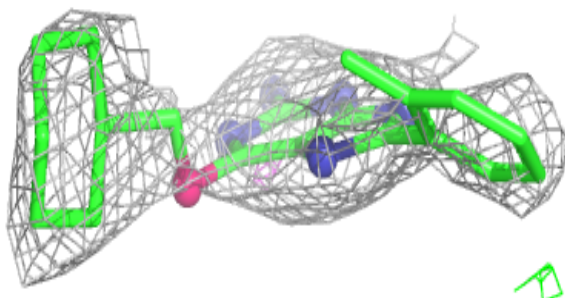
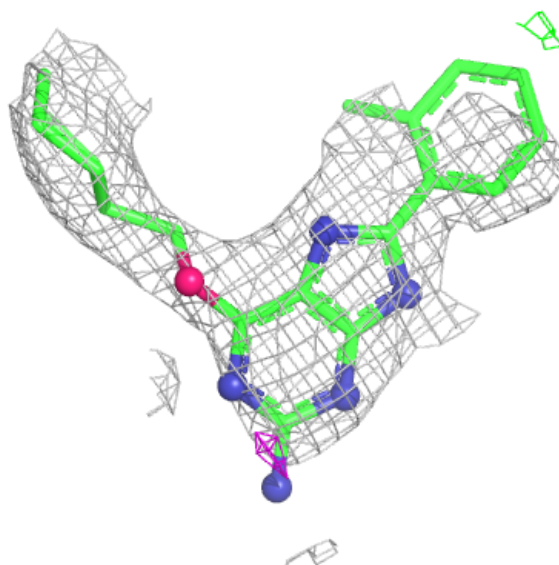
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	4QE	C	1297	25/25	0.76	0.18	80,87,93,94	0
3	4QE	A	1297	25/25	0.82	0.17	73,77,80,80	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.

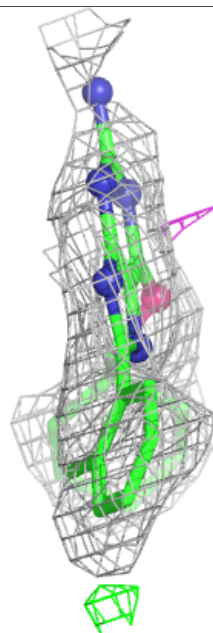
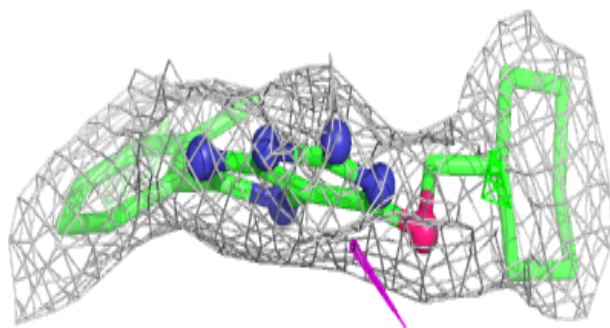
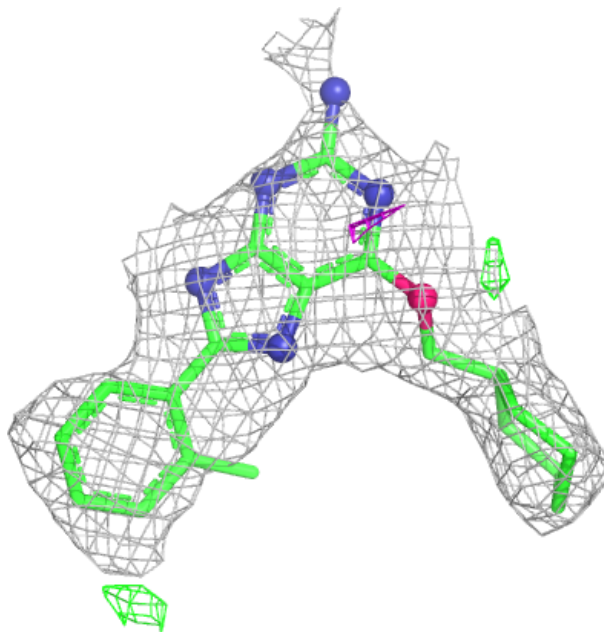
Electron density around 4QE C 1297:

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



Electron density around 4QE A 1297:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.