



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 2UZE / pdb_00002uze
Title : Crystal structure of human CDK2 complexed with a thiazolidinone inhibitor
Authors : Richardson, C.M.; Dokurno, P.; Murray, J.B.; Surgenor, A.E.
Deposited on : 2007-04-27
Resolution : 2.40 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

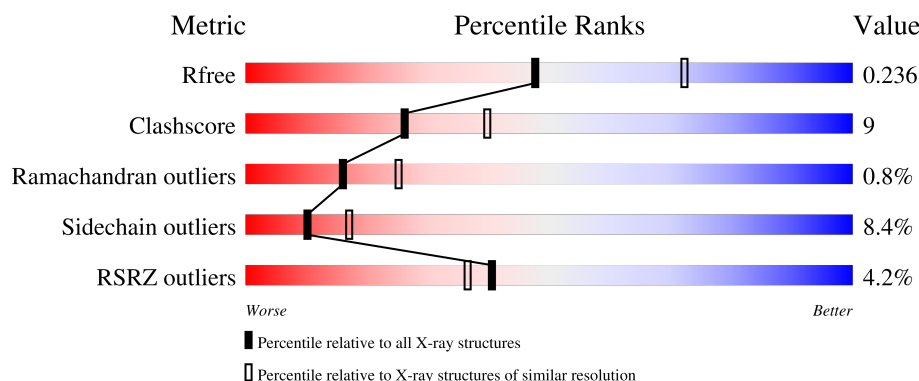
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	298	5% 72% 23% ...
1	C	298	6% 76% 20% ..
2	B	258	3% 77% 21% .
2	D	258	2% 81% 16% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	A	160	X	-	-	-
1	TPO	C	160	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9256 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.

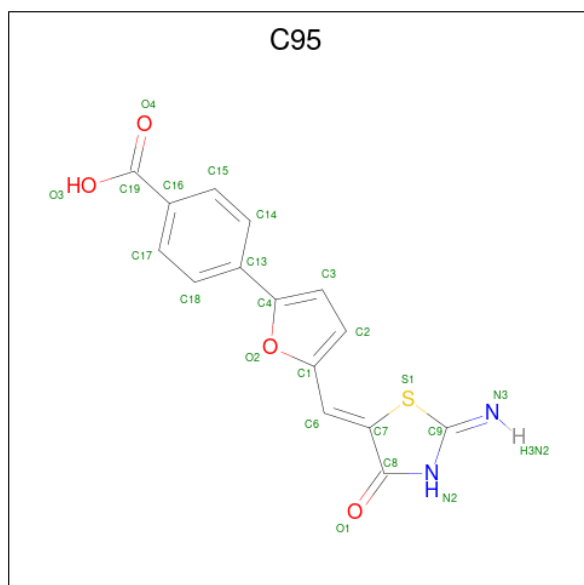
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	0	0
			2370	1541	400	420	1	8			
1	C	297	Total	C	N	O	P	S	0	0	1
			2378	1545	404	420	1	8			

- 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
			2084	1350	339	384	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

- Molecule 3 is 4-{5-[(Z)-(2-IMINO-4-OXO-1,3-THIAZOLIDIN-5-YLIDENE)METHYL]FURAN-2-YL}BENZOIC ACID (CCD ID: C95) (formula: C₁₅H₁₀N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	15	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			22	15	2	4	1		

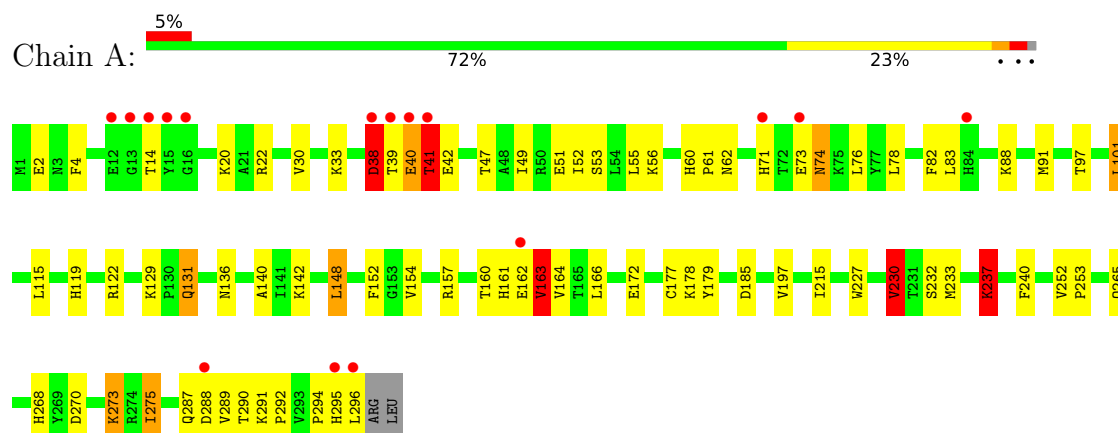
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	81	Total	O	0	0
			81	81		
4	C	75	Total	O	0	0
			75	75		
4	D	72	Total	O	0	0
			72	72		

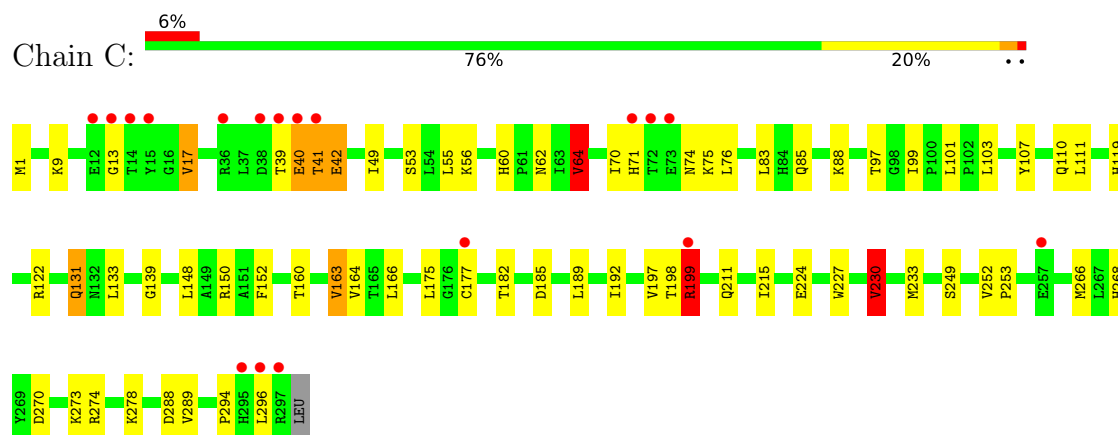
3 Residue-property plots

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.

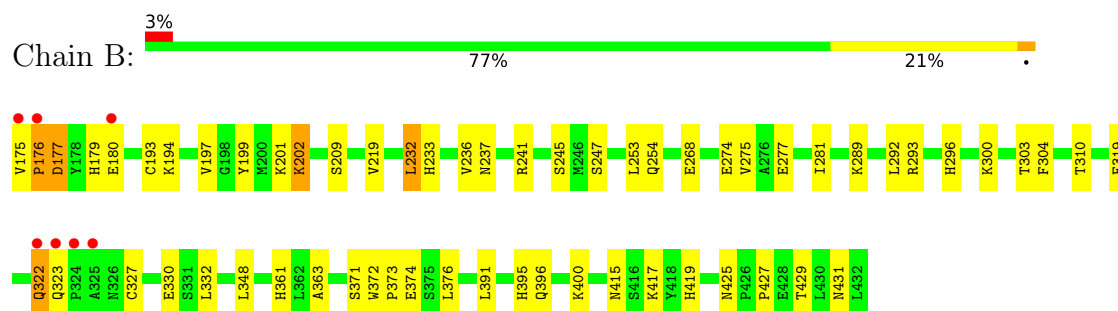
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



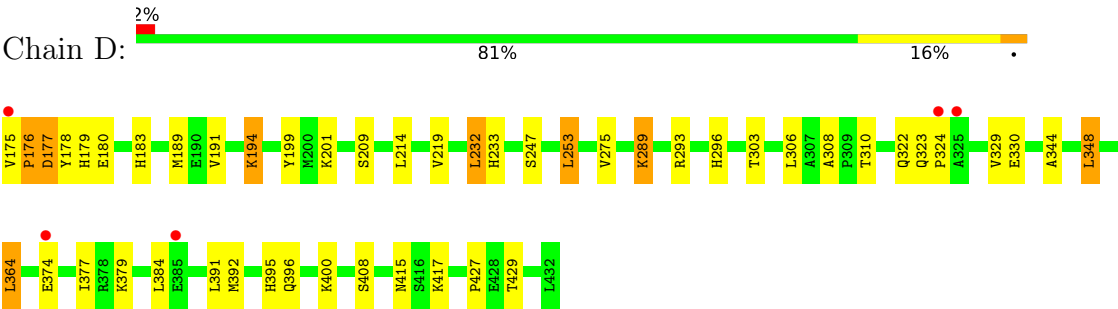
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 2: CYCLIN A2



● Molecule 2: CYCLIN A2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.63Å 73.44Å 153.03Å 90.00° 129.54° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.5 (20.00-2.40) 89.4 (20.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.243 0.191 , 0.236	Depositor DCC
R_{free} test set	3234 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9256	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: C95, TPO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.99	3/2420 (0.1%)	1.12	11/3285 (0.3%)
1	C	0.99	2/2428 (0.1%)	1.12	10/3295 (0.3%)
2	B	0.94	0/2134	1.14	1/2897 (0.0%)
2	D	0.92	0/2134	1.12	4/2897 (0.1%)
All	All	0.96	5/9116 (0.1%)	1.13	26/12374 (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	1	1
1	C	1	1
All	All	2	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	THR	CA-CB	6.55	1.61	1.53
1	C	296	LEU	C-N	-6.37	1.24	1.33
1	A	289	VAL	CA-CB	6.34	1.61	1.54
1	A	275	ILE	CA-CB	5.82	1.60	1.54
1	A	215	ILE	CA-CB	5.17	1.60	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CB-CA-C	-9.21	100.09	111.88
1	C	230	VAL	CB-CA-C	-8.88	100.15	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	PRO	N-CA-C	7.23	119.53	110.70
1	A	42	GLU	N-CA-C	7.16	122.02	113.28
1	C	13	GLY	N-CA-C	-6.83	102.06	112.51
1	C	64	VAL	CB-CA-C	-6.78	100.32	111.51
1	A	230	VAL	N-CA-CB	6.46	117.68	110.51
2	D	308	ALA	CA-C-N	6.21	125.97	119.76
2	D	308	ALA	C-N-CA	6.21	125.97	119.76
1	A	237	LYS	CA-C-N	-6.06	113.39	120.12
1	A	237	LYS	C-N-CA	-6.06	113.39	120.12
1	A	253	PRO	N-CA-C	5.88	117.87	110.70
1	A	163	VAL	N-CA-C	5.85	116.71	108.17
2	D	408	SER	N-CA-C	5.82	118.37	111.33
1	C	289	VAL	N-CA-C	5.81	116.92	109.30
1	C	270	ASP	CA-C-N	5.70	125.55	119.28
1	C	270	ASP	C-N-CA	5.70	125.55	119.28
1	C	85	GLN	N-CA-C	5.69	116.06	108.38
1	A	230	VAL	N-CA-C	5.49	116.12	110.36
1	C	296	LEU	O-C-N	-5.40	114.36	123.00
1	A	101	LEU	CA-C-N	-5.33	113.42	119.28
1	A	101	LEU	C-N-CA	-5.33	113.42	119.28
1	A	289	VAL	N-CA-C	5.16	115.75	109.30
2	B	236	VAL	N-CA-C	5.15	115.87	110.62
1	C	224	GLU	N-CA-C	5.04	117.50	111.71
2	D	189	MET	N-CA-C	5.04	116.85	111.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	160	TPO	CB
1	C	160	TPO	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	ASP	Peptide
1	C	40	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	2370	0	2404	59	0
1	C	2378	0	2418	53	0
2	B	2084	0	2107	34	0
2	D	2084	0	2107	31	0
3	A	22	0	8	1	0
3	C	22	0	8	1	0
4	A	68	0	0	12	0
4	B	81	0	0	4	0
4	C	75	0	0	15	0
4	D	72	0	0	9	0
All	All	9256	0	9052	170	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 (170) 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:B:176:PRO:HD2	2:B:179:HIS:CE1	1.51	1.45
1:C:64:VAL:HG23	4:C:2016:HOH:O	1.55	1.06
1:C:88:LYS:HE3	1:C:131:GLN:NE2	1.71	1.03
1:C:177:CYS:HB2	4:C:2049:HOH:O	1.59	1.02
2:B:176:PRO:CD	2:B:179:HIS:CE1	2.44	0.99
1:A:177:CYS:HB3	4:A:2040:HOH:O	1.60	0.99
1:A:74:ASN:HD22	1:A:74:ASN:H	0.99	0.94
1:A:74:ASN:H	1:A:74:ASN:ND2	1.67	0.91
1:C:64:VAL:CG2	4:C:2016:HOH:O	2.09	0.90
1:A:230:VAL:HA	1:A:233:MET:HE2	1.55	0.87
2:B:415:ASN:HB3	4:B:2079:HOH:O	1.75	0.86
1:C:233:MET:SD	4:C:2049:HOH:O	2.35	0.84
1:C:198:THR:O	1:C:199:ARG:HB3	1.79	0.82
1:A:74:ASN:HD22	1:A:74:ASN:N	1.78	0.81
2:B:395:HIS:HE1	2:B:427:PRO:O	1.63	0.80
1:C:88:LYS:CE	1:C:131:GLN:NE2	2.45	0.80
2:B:176:PRO:HD2	2:B:179:HIS:HE1	1.41	0.77
2:D:176:PRO:HD2	2:D:179:HIS:CE1	2.19	0.77
1:A:233:MET:SD	4:A:2039:HOH:O	2.42	0.77
1:A:60:HIS:HD2	1:A:62:ASN:H	1.33	0.77
1:A:227:TRP:O	1:A:230:VAL:HG22	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:HB3	4:C:2022:HOH:O	1.86	0.75
1:A:14:THR:HB	4:A:2023:HOH:O	1.86	0.75
1:A:177:CYS:HB2	4:A:2039:HOH:O	1.86	0.74
1:A:61:PRO:O	1:A:142:LYS:HE2	1.87	0.73
1:C:101:LEU:CB	4:C:2022:HOH:O	2.36	0.72
1:A:60:HIS:CD2	1:A:62:ASN:H	2.09	0.70
1:A:39:THR:O	1:A:40:GLU:CB	2.41	0.69
1:C:60:HIS:CD2	1:C:62:ASN:H	2.11	0.68
1:C:88:LYS:CE	1:C:131:GLN:HE22	2.04	0.68
1:A:197:VAL:HG11	1:A:252:VAL:HG22	1.77	0.66
1:C:9:LYS:HD2	1:C:17:VAL:HG11	1.77	0.65
2:B:319:PHE:O	2:B:322:GLN:HG3	1.96	0.65
1:A:252:VAL:HG13	1:A:252:VAL:O	1.97	0.65
1:C:227:TRP:O	1:C:230:VAL:HG22	1.97	0.64
1:A:268:HIS:CD2	4:A:2057:HOH:O	2.49	0.64
1:C:230:VAL:HG12	1:C:233:MET:HE2	1.80	0.64
2:D:233:HIS:HD2	4:D:2039:HOH:O	1.81	0.64
1:A:38:ASP:N	1:A:38:ASP:OD1	2.30	0.64
1:A:88:LYS:HA	1:A:91:MET:HE2	1.78	0.64
1:A:177:CYS:CB	4:A:2039:HOH:O	2.42	0.63
1:C:175:LEU:HD13	1:C:233:MET:HE3	1.81	0.63
2:B:322:GLN:HB3	4:B:2046:HOH:O	1.98	0.63
1:A:131:GLN:HG3	4:A:2021:HOH:O	1.98	0.63
1:C:60:HIS:HD2	1:C:62:ASN:H	1.48	0.62
1:C:88:LYS:HE3	1:C:131:GLN:HE22	1.58	0.62
1:C:42:GLU:OE1	2:D:275:VAL:HG23	2.00	0.62
1:A:101:LEU:O	1:A:101:LEU:HG	1.99	0.60
2:D:180:GLU:OE2	2:D:379:LYS:NZ	2.32	0.60
1:A:119:HIS:HD2	4:B:2007:HOH:O	1.84	0.60
1:C:198:THR:O	1:C:199:ARG:CB	2.49	0.59
1:A:71:HIS:CE1	2:B:296:HIS:CD2	2.91	0.59
1:A:14:THR:HG22	4:A:2006:HOH:O	2.01	0.59
1:A:230:VAL:HA	1:A:233:MET:CE	2.30	0.58
1:A:56:LYS:NZ	2:B:303:THR:O	2.36	0.58
1:C:64:VAL:CB	4:C:2016:HOH:O	2.48	0.57
1:C:9:LYS:HD2	1:C:17:VAL:CG1	2.34	0.57
1:C:64:VAL:HB	4:C:2016:HOH:O	2.04	0.57
1:A:172:GLU:O	1:A:177:CYS:HB2	2.05	0.57
1:C:1:MET:HG2	1:C:70:ILE:HG21	1.86	0.56
1:C:101:LEU:HB2	4:C:2022:HOH:O	2.04	0.56
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:GLN:NE2	2:B:330:GLU:OE2	2.39	0.55
1:A:20:LYS:HE3	1:A:82:PHE:CZ	2.41	0.55
2:B:296:HIS:HE1	2:B:300:LYS:NZ	2.05	0.55
3:C:1297:C95:S1	3:C:1297:C95:O2	2.65	0.54
3:A:1297:C95:S1	3:A:1297:C95:O2	2.66	0.54
2:B:233:HIS:HB3	2:B:310:THR:HB	1.89	0.54
2:D:233:HIS:HE1	4:D:2043:HOH:O	1.88	0.54
1:A:230:VAL:HG12	1:A:233:MET:HE3	1.89	0.54
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.43	0.53
1:A:177:CYS:SG	4:A:2039:HOH:O	2.59	0.53
2:B:193:CYS:O	2:B:241:ARG:HD2	2.08	0.53
4:C:2072:HOH:O	2:D:177:ASP:HB3	2.09	0.52
2:B:395:HIS:CE1	2:B:427:PRO:O	2.54	0.52
1:C:227:TRP:CE3	1:C:230:VAL:HG13	2.45	0.52
1:A:161:HIS:HD2	4:A:2041:HOH:O	1.93	0.52
1:A:38:ASP:OD2	1:A:41:THR:HB	2.11	0.51
1:C:101:LEU:HB2	4:C:2008:HOH:O	2.09	0.51
1:C:197:VAL:HG11	1:C:252:VAL:HG22	1.92	0.51
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.94	0.51
1:A:252:VAL:O	1:A:252:VAL:CG1	2.58	0.51
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.46	0.51
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.91	0.51
1:A:230:VAL:CG1	1:A:233:MET:CE	2.89	0.51
2:B:327:CYS:HB3	2:B:419:HIS:CE1	2.47	0.50
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.93	0.50
1:C:175:LEU:HD13	1:C:233:MET:CE	2.41	0.50
2:D:396:GLN:HE21	2:D:400:LYS:NZ	2.09	0.50
2:D:324:PRO:HB2	4:D:2042:HOH:O	2.12	0.50
1:A:4:PHE:CE1	1:A:30:VAL:HG21	2.46	0.49
1:A:14:THR:HG21	1:A:148:LEU:HD22	1.92	0.49
1:A:227:TRP:CH2	1:A:233:MET:HE1	2.48	0.49
1:C:252:VAL:O	1:C:252:VAL:HG13	2.12	0.49
2:D:178:TYR:HB2	4:D:2007:HOH:O	2.11	0.49
1:C:133:LEU:HD11	1:C:192:ILE:HD13	1.94	0.49
1:A:53:SER:HB3	2:B:304:PHE:O	2.13	0.49
1:A:237:LYS:HD3	1:A:240:PHE:CE1	2.48	0.48
2:B:275:VAL:HG21	2:B:292:LEU:HD21	1.94	0.48
1:A:88:LYS:HA	1:A:91:MET:CE	2.44	0.48
1:C:163:VAL:HG22	4:C:2033:HOH:O	2.13	0.48
1:A:136:ASN:ND2	1:A:140:ALA:HB3	2.29	0.48
1:A:178:LYS:HD3	1:A:179:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LYS:NZ	2:D:303:THR:O	2.42	0.48
1:C:268:HIS:CD2	4:C:2063:HOH:O	2.66	0.47
1:A:197:VAL:CG1	1:A:252:VAL:HG22	2.44	0.47
2:D:395:HIS:HE1	2:D:427:PRO:O	1.97	0.47
1:A:115:LEU:HD21	1:A:185:ASP:HB3	1.97	0.47
1:C:230:VAL:CG1	1:C:233:MET:HE2	2.44	0.47
2:D:415:ASN:HB3	4:D:2070:HOH:O	2.15	0.47
1:C:71:HIS:CE1	2:D:296:HIS:CD2	3.03	0.47
4:C:2072:HOH:O	2:D:177:ASP:CB	2.63	0.46
2:B:274:GLU:HB2	2:B:277:GLU:HG3	1.97	0.46
1:A:163:VAL:HG22	4:A:2019:HOH:O	2.16	0.46
2:B:202:LYS:HA	2:B:202:LYS:HD2	1.67	0.46
1:C:227:TRP:CD2	1:C:230:VAL:HG13	2.50	0.46
2:D:392:MET:HA	2:D:392:MET:HE2	1.98	0.46
1:A:157:ARG:NH1	2:B:268:GLU:OE2	2.39	0.45
2:D:175:VAL:HG22	4:D:2003:HOH:O	2.16	0.45
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.51	0.45
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.98	0.45
2:B:289:LYS:O	2:B:293:ARG:HG3	2.16	0.45
2:D:322:GLN:NE2	2:D:330:GLU:OE2	2.50	0.45
2:D:233:HIS:HB3	2:D:310:THR:HB	1.97	0.45
1:C:119:HIS:CD2	1:C:182:THR:HB	2.52	0.45
1:C:227:TRP:CH2	1:C:233:MET:HE1	2.52	0.45
2:D:289:LYS:HG2	2:D:293:ARG:HH21	1.82	0.45
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.98	0.45
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.51	0.45
4:A:2066:HOH:O	2:B:177:ASP:HB3	2.16	0.45
1:C:211:GLN:O	1:C:215:ILE:HG13	2.18	0.44
2:B:176:PRO:CD	2:B:179:HIS:HE1	2.11	0.44
1:A:290:THR:C	1:A:292:PRO:HD3	2.41	0.44
2:B:237:ASN:OD1	2:B:241:ARG:HD3	2.18	0.44
1:A:52:ILE:O	1:A:56:LYS:HG2	2.17	0.44
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.53	0.44
1:A:294:PRO:C	1:A:296:LEU:H	2.24	0.44
2:D:329:VAL:HG11	2:D:364:LEU:HD13	2.00	0.44
1:A:265:GLN:NE2	1:A:275:ILE:HD12	2.33	0.43
2:B:219:VAL:HG22	2:B:232:LEU:HD11	2.00	0.43
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.02	0.43
1:A:33:LYS:NZ	1:A:51:GLU:OE1	2.50	0.43
2:D:183:HIS:HE1	4:D:2011:HOH:O	2.01	0.42
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.54	0.42
2:D:176:PRO:HG2	2:D:179:HIS:CD2	2.55	0.42
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.34	0.42
1:C:107:TYR:O	1:C:111:LEU:HG	2.20	0.42
2:D:322:GLN:HB3	4:D:2041:HOH:O	2.19	0.42
1:A:270:ASP:HB3	1:A:273:LYS:HB2	2.02	0.42
1:C:101:LEU:O	1:C:101:LEU:HD12	2.19	0.42
1:A:230:VAL:HG13	1:A:233:MET:CE	2.50	0.41
1:C:175:LEU:CD1	1:C:233:MET:HE3	2.46	0.41
1:C:99:ILE:HG23	1:C:103:LEU:HD23	2.02	0.41
2:D:219:VAL:HG22	2:D:232:LEU:HD11	2.02	0.41
1:C:273:LYS:HD2	4:C:2064:HOH:O	2.20	0.41
2:D:374:GLU:OE1	4:D:2050:HOH:O	2.21	0.41
2:B:199:TYR:C	2:B:199:TYR:CD1	2.98	0.41
2:D:191:VAL:O	2:D:194:LYS:HG3	2.20	0.41
2:B:254:GLN:NE2	4:B:2032:HOH:O	2.51	0.41
2:D:214:LEU:HD22	2:D:253:LEU:HD22	2.03	0.41
2:B:296:HIS:HE1	2:B:300:LYS:HZ1	1.68	0.41
1:C:175:LEU:CD1	1:C:233:MET:CE	2.98	0.41
1:C:230:VAL:HA	1:C:233:MET:HE2	2.03	0.40
1:C:49:ILE:HG23	2:D:306:LEU:HD12	2.02	0.40
2:D:199:TYR:CD1	2:D:199:TYR:C	3.00	0.40
2:B:371:SER:O	2:B:372:TRP:C	2.64	0.40
2:B:373:PRO:HD2	2:B:376:LEU:HD12	2.03	0.40
2:B:396:GLN:HE21	2:B:400:LYS:NZ	2.19	0.40
1:C:266:MET:O	1:C:274:ARG:HD3	2.21	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	293/298 (98%)	281 (96%)	8 (3%)	4 (1%)	9	13
1	C	294/298 (99%)	281 (96%)	10 (3%)	3 (1%)	12	20
2	B	256/258 (99%)	253 (99%)	2 (1%)	1 (0%)	30	43
2	D	256/258 (99%)	253 (99%)	2 (1%)	1 (0%)	30	43
All	All	1099/1112 (99%)	1068 (97%)	22 (2%)	9 (1%)	16	25

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	164	VAL
1	C	164	VAL
1	A	40	GLU
1	C	199	ARG
1	A	162	GLU
2	B	176	PRO
1	C	39	THR
2	D	176	PRO

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	257/262 (98%)	233 (91%)	24 (9%)	8	14
1	C	258/262 (98%)	236 (92%)	22 (8%)	10	16
2	B	232/232 (100%)	211 (91%)	21 (9%)	9	14
2	D	232/232 (100%)	217 (94%)	15 (6%)	15	27
All	All	979/988 (99%)	897 (92%)	82 (8%)	10	17

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	22	ARG

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Mol	Chain	Res	Type
1	A	38	ASP
1	A	41	THR
1	A	47	THR
1	A	49	ILE
1	A	55	LEU
1	A	73	GLU
1	A	74	ASN
1	A	78	LEU
1	A	83	LEU
1	A	97	THR
1	A	131	GLN
1	A	148	LEU
1	A	163	VAL
1	A	166	LEU
1	A	230	VAL
1	A	232	SER
1	A	237	LYS
1	A	273	LYS
1	A	287	GLN
1	A	288	ASP
1	A	291	LYS
1	A	295	HIS
2	B	175	VAL
2	B	177	ASP
2	B	180	GLU
2	B	194	LYS
2	B	197	VAL
2	B	201	LYS
2	B	202	LYS
2	B	209	SER
2	B	232	LEU
2	B	245	SER
2	B	247	SER
2	B	253	LEU
2	B	281	ILE
2	B	322	GLN
2	B	323	GLN
2	B	348	LEU
2	B	374	GLU
2	B	417	LYS
2	B	425	ASN
2	B	429	THR

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Mol	Chain	Res	Type
2	B	431	ASN
1	C	17	VAL
1	C	40	GLU
1	C	41	THR
1	C	42	GLU
1	C	53	SER
1	C	55	LEU
1	C	64	VAL
1	C	74	ASN
1	C	75	LYS
1	C	83	LEU
1	C	97	THR
1	C	131	GLN
1	C	148	LEU
1	C	150	ARG
1	C	163	VAL
1	C	166	LEU
1	C	189	LEU
1	C	199	ARG
1	C	230	VAL
1	C	249	SER
1	C	278	LYS
1	C	288	ASP
2	D	177	ASP
2	D	194	LYS
2	D	201	LYS
2	D	209	SER
2	D	232	LEU
2	D	247	SER
2	D	253	LEU
2	D	289	LYS
2	D	323	GLN
2	D	348	LEU
2	D	364	LEU
2	D	384	LEU
2	D	391	LEU
2	D	417	LYS
2	D	429	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	62	ASN
1	A	71	HIS
1	A	74	ASN
1	A	85	GLN
1	A	119	HIS
1	A	265	GLN
1	A	272	ASN
2	B	179	HIS
2	B	183	HIS
2	B	254	GLN
2	B	296	HIS
2	B	312	ASN
2	B	317	GLN
2	B	395	HIS
2	B	396	GLN
2	B	419	HIS
1	C	59	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	85	GLN
1	C	119	HIS
1	C	131	GLN
1	C	265	GLN
1	C	268	HIS
2	D	183	HIS
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	395	HIS
2	D	396	GLN
2	D	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	C	160	1	8,10,11	1.01	0	10,14,16	2.57	3 (30%)
1	TPO	A	160	1	8,10,11	0.77	0	10,14,16	2.55	3 (30%)

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	1/1/3/4	6/9/11/13	-
1	TPO	A	160	1	1/1/3/4	4/9/11/13	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	P-OG1-CB	6.56	141.14	123.33
1	A	160	TPO	P-OG1-CB	5.23	137.53	123.33
1	A	160	TPO	CG2-CB-CA	4.90	122.81	113.26
1	C	160	TPO	CG2-CB-CA	3.59	120.25	113.26
1	A	160	TPO	O-C-CA	-2.07	119.44	124.77
1	C	160	TPO	O-C-CA	-2.02	119.58	124.77

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	160	TPO	CB
1	C	160	TPO	CB

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
1	A	160	TPO	C-CA-CB-CG2
1	A	160	TPO	O-C-CA-CB
1	C	160	TPO	N-CA-CB-CG2
1	C	160	TPO	N-CA-CB-OG1
1	C	160	TPO	C-CA-CB-CG2
1	C	160	TPO	O-C-CA-CB
1	C	160	TPO	CA-CB-OG1-P
1	A	160	TPO	N-CA-CB-CG2
1	C	160	TPO	CB-OG1-P-O3P

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](#)

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	C95	C	1297	-	24,24,24	1.92	5 (20%)	32,34,34	1.96	4 (12%)
3	C95	A	1297	-	24,24,24	1.70	5 (20%)	32,34,34	2.02	6 (18%)

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	C95	C	1297	-	-	0/12/24/24	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C95	A	1297	-	-	1/12/24/24	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1297	C95	C8-C7	-5.52	1.39	1.48
3	C	1297	C95	C9-S1	-4.75	1.67	1.74
3	A	1297	C95	C9-S1	-4.36	1.68	1.74
3	A	1297	C95	C8-C7	-3.81	1.42	1.48
3	C	1297	C95	O2-C4	-3.02	1.33	1.38
3	A	1297	C95	C6-C1	2.83	1.49	1.43
3	A	1297	C95	C7-S1	-2.72	1.67	1.73
3	C	1297	C95	O2-C1	-2.44	1.34	1.38
3	C	1297	C95	C6-C1	2.34	1.48	1.43
3	A	1297	C95	O2-C1	-2.18	1.34	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1297	C95	O2-C4-C13	6.74	124.71	116.73
3	C	1297	C95	O2-C4-C13	6.39	124.30	116.73
3	A	1297	C95	C1-C6-C7	-5.50	118.73	128.15
3	C	1297	C95	C1-C6-C7	-5.49	118.75	128.15
3	A	1297	C95	C6-C7-C8	3.07	125.40	121.25
3	C	1297	C95	C6-C7-C8	2.58	124.75	121.25
3	A	1297	C95	O2-C4-C3	-2.24	107.67	109.39
3	A	1297	C95	O3-C19-C16	2.19	120.45	114.84
3	A	1297	C95	C9-S1-C7	2.08	92.25	89.35
3	C	1297	C95	C7-C8-N2	2.02	111.84	110.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1297	C95	C1-C6-C7-C8

There are no ring outliers.

2 monomers are involved in 2 short contacts:

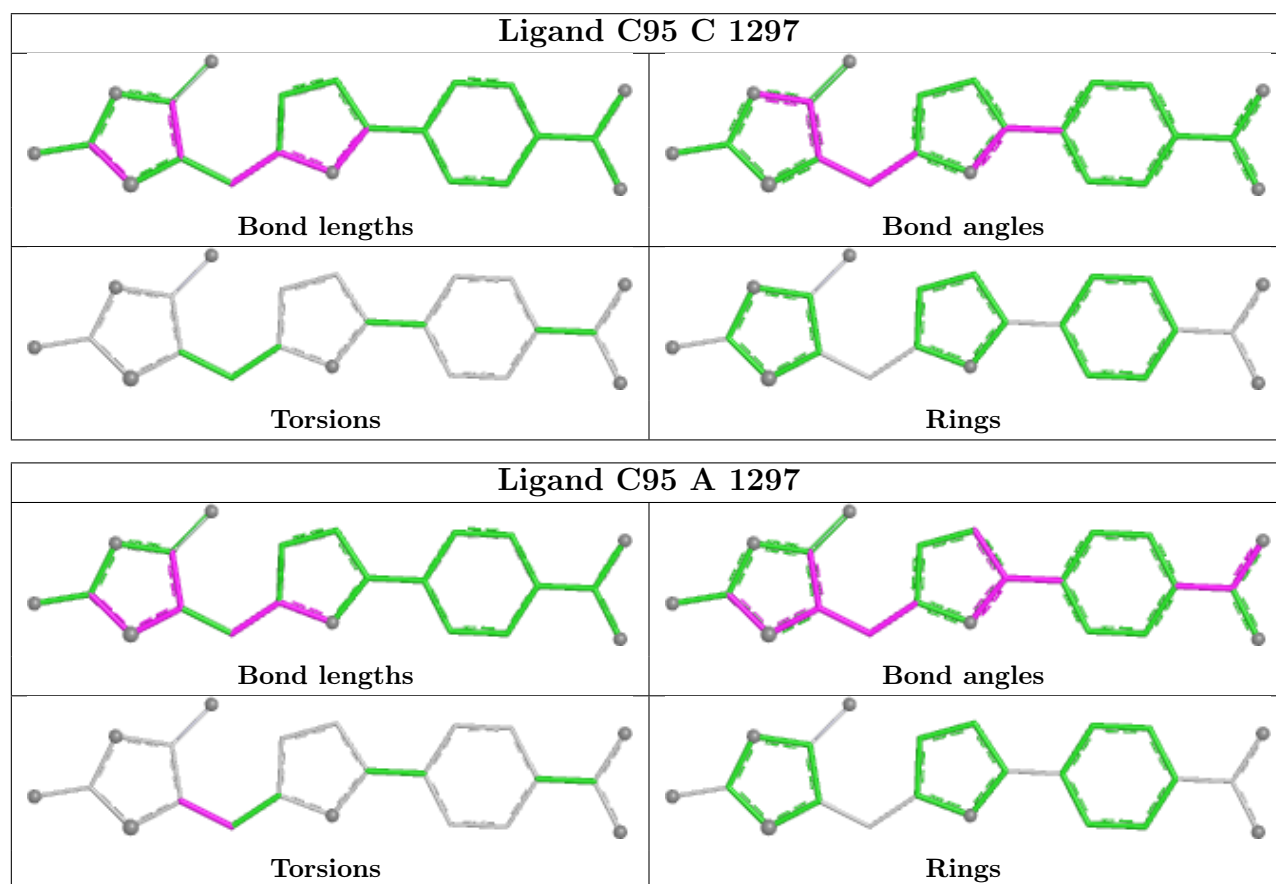
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	C95	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1297	C95	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 ⓘ

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	295/298 (98%)	-0.11	16 (5%)	31 28	13, 27, 52, 66	9 (3%)
1	C	296/298 (99%)	-0.05	18 (6%)	27 23	14, 27, 54, 67	10 (3%)
2	B	258/258 (100%)	-0.35	7 (2%)	56 52	14, 25, 43, 63	0
2	D	258/258 (100%)	-0.38	5 (1%)	66 62	14, 25, 44, 63	0
All	All	1107/1112 (99%)	-0.21	46 (4%)	40 36	13, 26, 51, 67	19 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	9.2
1	A	39	THR	6.4
2	B	175	VAL	6.3
1	C	14	THR	5.9
1	A	296	LEU	5.9
1	A	295	HIS	5.6
1	C	296	LEU	5.3
1	C	38	ASP	5.0
1	A	38	ASP	5.0
1	C	40	GLU	5.0
2	B	324	PRO	5.0
2	D	175	VAL	4.9
1	A	40	GLU	4.9
1	C	295	HIS	4.2
1	C	41	THR	4.0
1	C	13	GLY	4.0
2	B	176	PRO	3.9
1	A	41	THR	3.9
1	A	15	TYR	3.6
1	A	14	THR	3.5
2	D	324	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	15	TYR	3.4
1	C	12	GLU	3.3
1	C	72	THR	3.2
1	C	297	ARG	3.1
2	D	374	GLU	3.0
1	A	71	HIS	3.0
1	C	199	ARG	2.9
1	A	12	GLU	2.9
2	B	323	GLN	2.8
2	D	325	ALA	2.8
2	B	180	GLU	2.7
1	A	13	GLY	2.7
1	A	16	GLY	2.6
1	C	73	GLU	2.6
1	C	71	HIS	2.6
2	B	322	GLN	2.5
1	A	162	GLU	2.4
1	A	84	HIS	2.4
1	C	257	GLU	2.4
2	D	385	GLU	2.3
2	B	325	ALA	2.2
1	A	73	GLU	2.2
1	C	177	CYS	2.2
1	A	288	ASP	2.2
1	C	36	ARG	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	C	160	11/12	0.98	0.06	18,22,25,25	0
1	TPO	A	160	11/12	0.99	0.05	17,21,24,24	0

6.3 Carbohydrates [i](#)

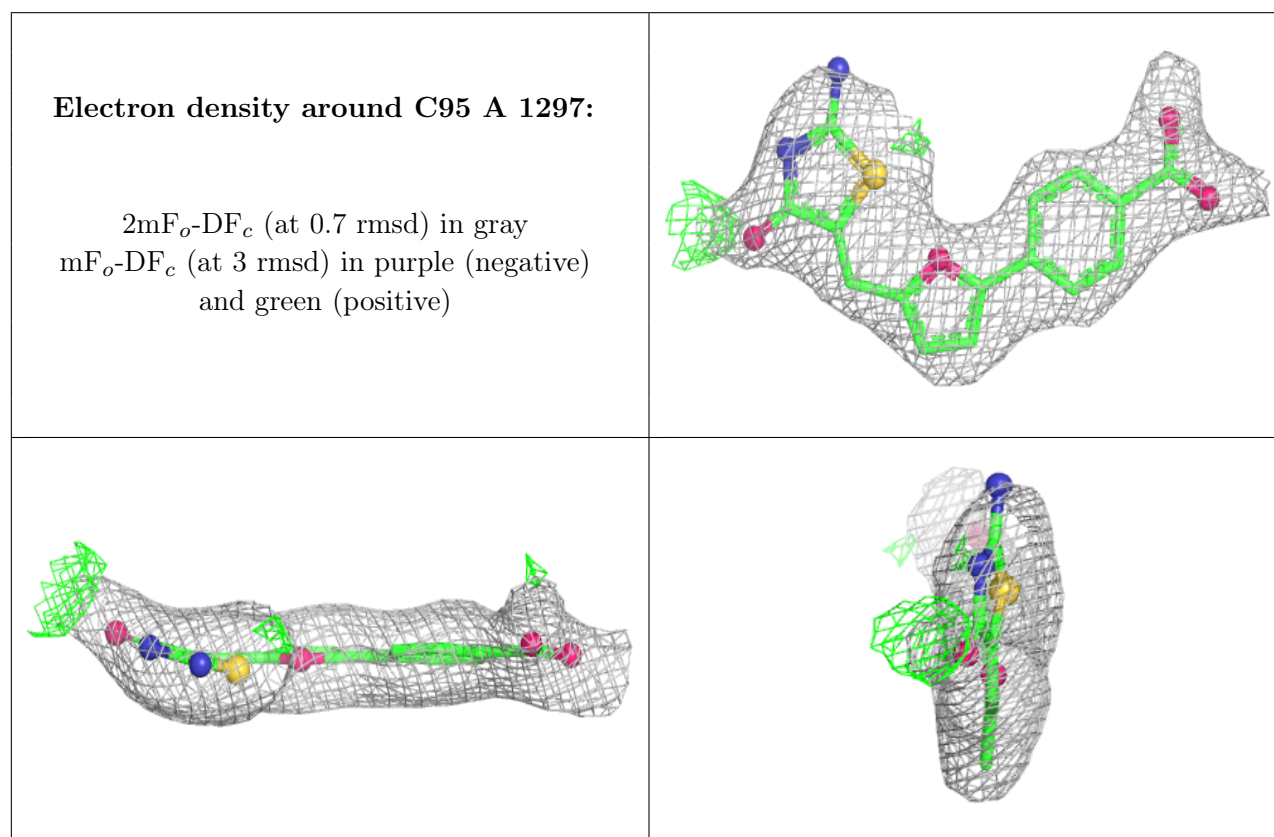
There are no oligosaccharides in this entry.

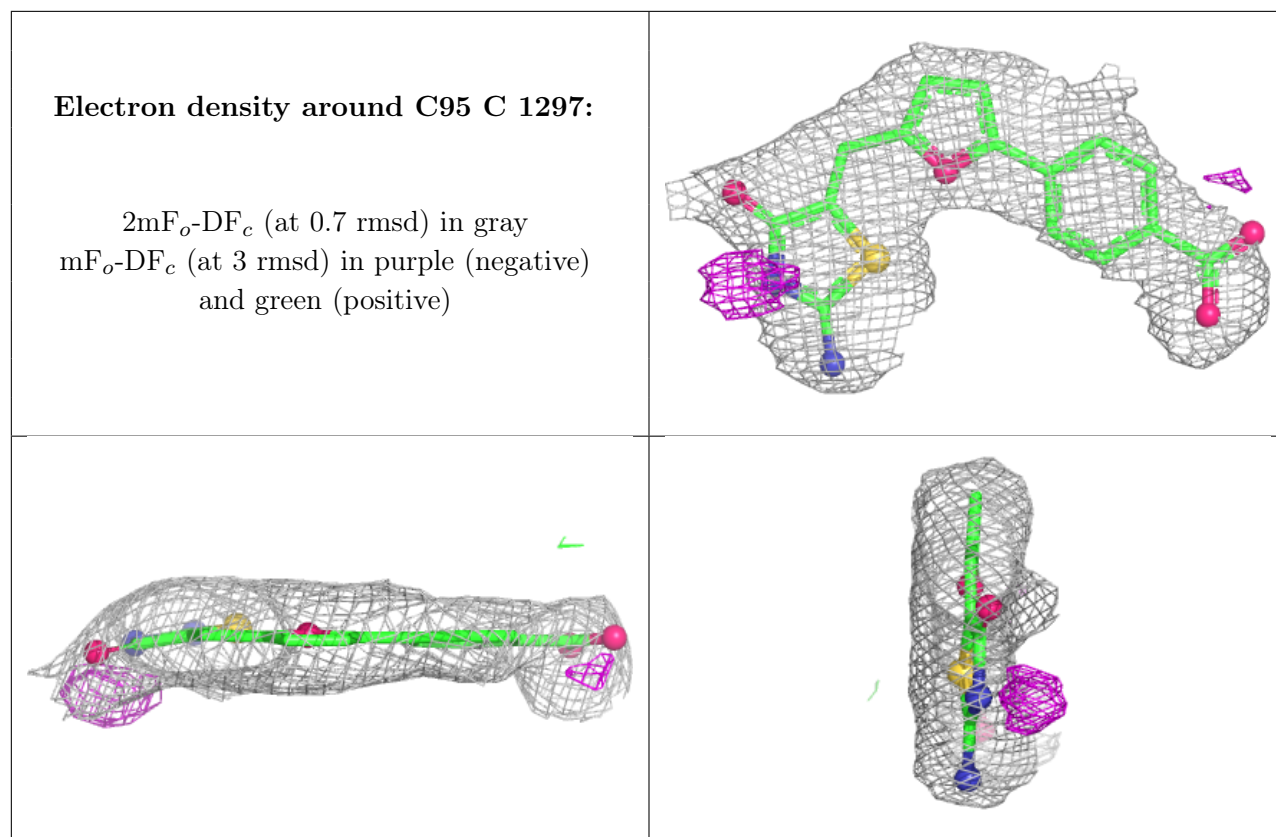
6.4 Ligands ⓘ

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	C95	A	1297	22/22	0.90	0.10	49,51,56,57	0
3	C95	C	1297	22/22	0.90	0.12	47,49,53,57	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.