



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:59 AM UTC

PDB ID : 2B54 / pdb_00002b54
Title : Human cyclin dependent kinase 2 (CKD2)complexed with DIN-232305
Authors : Chang, C.-C.
Deposited on : 2005-09-27
Resolution : 1.85 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 ⓘ](#)) 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

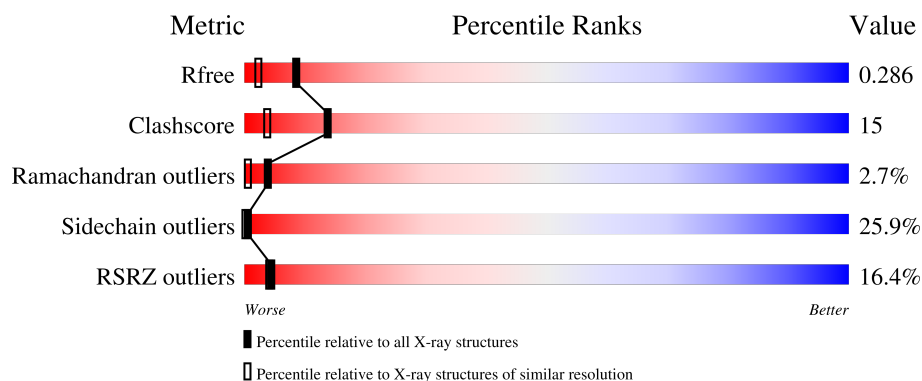
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	16% 40% 36% 16% 8%

2 Entry composition [i](#)

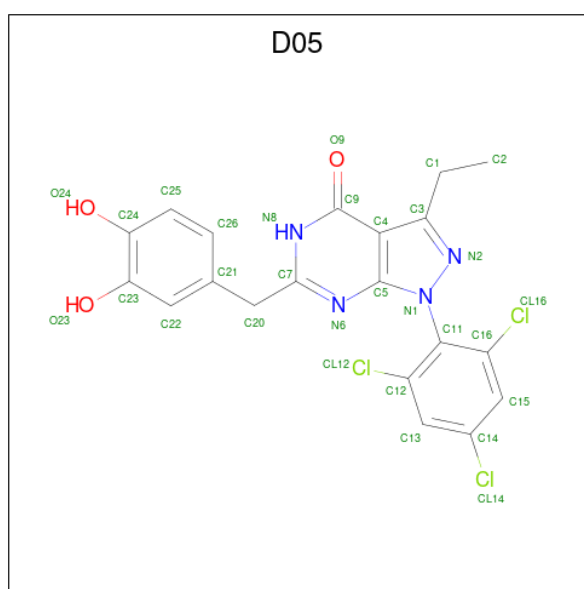
There are 3 unique types of molecules in this entry. The entry contains 3259 atoms, of which 725 are hydrogens and 0 are deuteriums.

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	298	Total	C	H	N	O	S	0	0	0
			2911	1559	513	408	423	8			

- Molecule 2 is 6-(3,4-DIHYDROXYBENZYL)-3-ETHYL-1-(2,4,6-TRICHLOROPHENYL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-4(5H)-ONE (CCD ID: D05) (formula: C₂₀H₁₅Cl₃N₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			30	20	3	4	3		

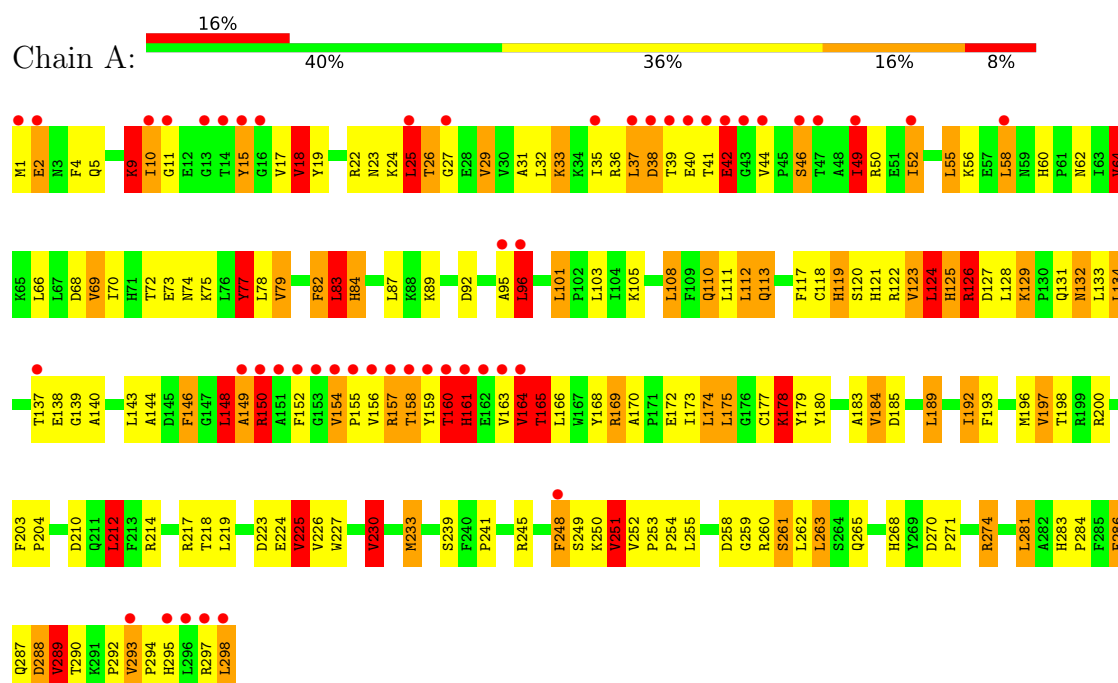
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	H	O	0
			318	212	106	

3 Residue-property plots [i](#)

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

• Molecule 1: Cell division protein kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.97Å 73.16Å 54.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.44 – 1.85 37.44 – 1.85	Depositor EDS
% Data completeness (in resolution range)	78.0 (37.44-1.85) 78.0 (37.44-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 1.84Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.158 , 0.263 (Not available) , 0.286	Depositor DCC
R_{free} test set	1976 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3259	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 6.82% 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: D05

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	1.30	13/2460 (0.5%)	2.21	117/3338 (3.5%)

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	11

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	HIS	CE1-NE2	6.06	1.38	1.32
1	A	268	HIS	ND1-CE1	5.54	1.38	1.32
1	A	125	HIS	CG-CD2	5.45	1.41	1.35
1	A	119	HIS	CE1-NE2	5.42	1.38	1.32
1	A	268	HIS	CE1-NE2	5.41	1.38	1.32
1	A	283	HIS	CE1-NE2	5.41	1.38	1.32
1	A	119	HIS	CG-CD2	5.41	1.41	1.35
1	A	119	HIS	ND1-CE1	5.39	1.38	1.32
1	A	125	HIS	ND1-CE1	5.37	1.38	1.32
1	A	161	HIS	CE1-NE2	5.31	1.37	1.32
1	A	233	MET	C-N	5.17	1.40	1.34
1	A	295	HIS	CE1-NE2	5.02	1.37	1.32
1	A	18	VAL	CA-C	-5.00	1.46	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	VAL	CB-CA-C	11.04	120.84	110.13
1	A	161	HIS	CA-CB-CG	-10.44	103.36	113.80
1	A	293	VAL	N-CA-CB	-9.34	102.47	112.37
1	A	9	LYS	CA-C-N	-9.05	108.55	122.76
1	A	9	LYS	C-N-CA	-9.05	108.55	122.76
1	A	184	VAL	CA-CB-CG1	8.78	125.33	110.40
1	A	184	VAL	N-CA-CB	-8.60	99.72	110.47
1	A	161	HIS	N-CA-C	8.30	123.76	111.81
1	A	172	GLU	CA-CB-CG	8.27	130.63	114.10
1	A	124	LEU	CB-CA-C	8.21	124.49	109.71
1	A	122	ARG	CA-C-N	-7.91	113.39	123.19
1	A	122	ARG	C-N-CA	-7.91	113.39	123.19
1	A	133	LEU	CA-C-N	-7.81	110.71	122.74
1	A	133	LEU	C-N-CA	-7.81	110.71	122.74
1	A	124	LEU	N-CA-CB	-7.47	99.35	110.85
1	A	154	VAL	N-CA-C	7.30	116.99	108.96
1	A	123	VAL	CA-C-N	-7.26	110.14	122.92
1	A	123	VAL	C-N-CA	-7.26	110.14	122.92
1	A	27	GLY	CA-C-N	-7.21	110.39	122.64
1	A	27	GLY	C-N-CA	-7.21	110.39	122.64
1	A	96	LEU	N-CA-C	6.97	121.02	112.23
1	A	251	VAL	CB-CA-C	6.83	120.55	111.94
1	A	230	VAL	CA-CB-CG2	6.67	121.74	110.40
1	A	292	PRO	CA-C-N	-6.65	117.54	123.33
1	A	292	PRO	C-N-CA	-6.65	117.54	123.33
1	A	178	LYS	CB-CG-CD	6.60	126.49	111.30
1	A	118	CYS	O-C-N	6.60	128.86	122.07
1	A	78	LEU	CA-C-N	-6.55	114.35	123.13
1	A	78	LEU	C-N-CA	-6.55	114.35	123.13
1	A	79	VAL	CB-CA-C	6.48	119.41	110.99
1	A	239	SER	N-CA-C	6.44	120.74	113.01
1	A	160	THR	CA-C-N	-6.41	110.41	122.27
1	A	160	THR	C-N-CA	-6.41	110.41	122.27
1	A	149	ALA	CA-C-N	6.39	133.74	121.54
1	A	149	ALA	C-N-CA	6.39	133.74	121.54
1	A	217	ARG	CA-C-N	6.38	129.12	120.44
1	A	217	ARG	C-N-CA	6.38	129.12	120.44
1	A	29	VAL	CA-CB-CG1	6.33	121.17	110.40
1	A	193	PHE	N-CA-C	6.30	118.67	111.11
1	A	49	ILE	N-CA-C	6.29	117.04	110.62
1	A	230	VAL	CB-CA-C	-6.28	100.99	111.29
1	A	258	ASP	CA-CB-CG	6.25	118.84	112.60
1	A	92	ASP	N-CA-C	6.24	118.88	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	LEU	CA-C-N	-6.19	111.98	120.28
1	A	87	LEU	C-N-CA	-6.19	111.98	120.28
1	A	140	ALA	N-CA-C	6.18	118.35	109.14
1	A	248	PHE	N-CA-C	6.17	118.81	111.71
1	A	123	VAL	CA-C-O	6.14	126.99	120.48
1	A	95	ALA	N-CA-C	6.06	117.89	111.28
1	A	226	VAL	CA-C-N	-6.05	114.69	122.98
1	A	226	VAL	C-N-CA	-6.05	114.69	122.98
1	A	83	LEU	CD1-CG-CD2	-6.00	97.60	110.80
1	A	289	VAL	CB-CA-C	-5.92	101.93	111.59
1	A	172	GLU	CB-CA-C	-5.87	100.70	110.68
1	A	233	MET	CA-C-O	-5.87	114.59	120.64
1	A	289	VAL	N-CA-CB	5.83	117.94	110.13
1	A	196	MET	CA-C-N	-5.82	113.12	120.56
1	A	196	MET	C-N-CA	-5.82	113.12	120.56
1	A	68	ASP	CA-C-N	5.81	132.43	121.97
1	A	68	ASP	C-N-CA	5.81	132.43	121.97
1	A	204	PRO	CA-C-N	-5.75	114.45	120.31
1	A	204	PRO	C-N-CA	-5.75	114.45	120.31
1	A	148	LEU	O-C-N	5.74	128.21	122.12
1	A	4	PHE	CA-CB-CG	-5.72	108.08	113.80
1	A	74	ASN	CA-CB-CG	-5.70	106.90	112.60
1	A	295	HIS	CA-C-N	-5.70	110.57	122.03
1	A	295	HIS	C-N-CA	-5.70	110.57	122.03
1	A	230	VAL	N-CA-CB	5.66	120.56	111.23
1	A	70	ILE	N-CA-CB	-5.65	105.80	111.90
1	A	251	VAL	CA-C-N	-5.65	111.68	122.13
1	A	251	VAL	C-N-CA	-5.65	111.68	122.13
1	A	2	GLU	N-CA-C	5.64	119.78	113.01
1	A	29	VAL	N-CA-CB	-5.64	104.57	111.00
1	A	148	LEU	CB-CA-C	-5.64	101.43	110.79
1	A	289	VAL	N-CA-C	5.63	116.97	109.37
1	A	113	GLN	N-CA-CB	-5.60	101.60	109.94
1	A	290	THR	CA-C-N	-5.57	116.83	122.74
1	A	290	THR	C-N-CA	-5.57	116.83	122.74
1	A	260	ARG	N-CA-C	5.55	118.26	111.82
1	A	225	VAL	CA-CB-CG2	5.55	119.84	110.40
1	A	192	ILE	CA-CB-CG1	5.55	119.84	110.40
1	A	146	PHE	CA-CB-CG	-5.53	108.27	113.80
1	A	197	VAL	N-CA-C	5.51	115.71	110.53
1	A	64	VAL	CA-CB-CG2	5.49	119.73	110.40
1	A	261	SER	O-C-N	5.46	127.90	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	192	ILE	CA-C-N	5.40	127.83	120.54
1	A	192	ILE	C-N-CA	5.40	127.83	120.54
1	A	198	THR	N-CA-C	5.35	119.53	112.89
1	A	110	GLN	N-CA-C	5.33	116.77	111.07
1	A	224	GLU	N-CA-C	5.29	119.36	113.01
1	A	260	ARG	CA-CB-CG	-5.28	103.54	114.10
1	A	120	SER	O-C-N	5.25	127.69	122.12
1	A	26	THR	N-CA-C	5.24	117.07	111.36
1	A	79	VAL	CA-CB-CG2	5.24	119.31	110.40
1	A	265	GLN	N-CA-C	5.23	117.72	111.71
1	A	129	LYS	CB-CA-C	5.22	118.06	109.97
1	A	212	LEU	N-CA-C	5.22	117.39	111.02
1	A	137	THR	N-CA-C	5.21	119.27	113.01
1	A	25	LEU	CA-CB-CG	5.21	134.52	116.30
1	A	286	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	46	SER	O-C-N	5.15	128.07	122.20
1	A	241	PRO	CA-C-N	-5.12	115.39	122.30
1	A	241	PRO	C-N-CA	-5.12	115.39	122.30
1	A	118	CYS	CA-C-N	5.10	127.11	120.28
1	A	118	CYS	C-N-CA	5.10	127.11	120.28
1	A	203	PHE	CB-CA-C	-5.10	102.74	111.15
1	A	250	LYS	CA-C-O	5.08	125.79	119.79
1	A	69	VAL	CB-CA-C	-5.07	102.97	111.29
1	A	218	THR	CA-C-N	-5.05	114.20	122.54
1	A	218	THR	C-N-CA	-5.05	114.20	122.54
1	A	230	VAL	N-CA-C	5.03	119.81	109.34
1	A	118	CYS	N-CA-C	5.02	116.44	111.07
1	A	84	HIS	CA-C-O	-5.02	115.10	120.42
1	A	101	LEU	N-CA-C	5.01	120.89	109.81
1	A	261	SER	N-CA-CB	5.01	117.48	110.12
1	A	288	ASP	N-CA-C	5.01	118.97	113.21

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ARG	Sidechain
1	A	157	ARG	Peptide
1	A	158	THR	Peptide
1	A	160	THR	Peptide
1	A	161	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	169	ARG	Sidechain
1	A	22	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	274	ARG	Sidechain
1	A	42	GLU	Peptide
1	A	77	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	2398	513	2450	71	2
2	A	30	0	15	2	0
3	A	106	212	0	2	1
All	All	2534	725	2465	71	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLN:HG3	1:A:288:ASP:H	1.44	0.82
1:A:18:VAL:HB	1:A:33:LYS:HD3	1.67	0.76
1:A:227:TRP:O	1:A:230:VAL:HG22	1.94	0.67
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.78	0.66
1:A:37:LEU:H	1:A:37:LEU:HD13	1.60	0.65
1:A:255:LEU:HD22	1:A:259:GLY:HA3	1.80	0.63
1:A:286:PHE:O	1:A:289:VAL:HG22	2.00	0.61
1:A:18:VAL:HB	1:A:33:LYS:CD	2.31	0.60
1:A:148:LEU:C	1:A:150:ARG:H	2.09	0.60
1:A:129:LYS:HG2	1:A:132:ASN:HD21	1.66	0.60
1:A:297:ARG:O	1:A:298:LEU:HD13	2.03	0.59
1:A:82:PHE:O	1:A:83:LEU:HD23	2.03	0.58
1:A:125:HIS:HE1	1:A:144:ALA:O	1.86	0.57
1:A:248:PHE:HA	1:A:251:VAL:HG13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD22	1:A:26:THR:HG23	1.85	0.57
1:A:134:LEU:HD22	1:A:144:ALA:HB2	1.86	0.56
1:A:125:HIS:HD2	1:A:127:ASP:H	1.53	0.55
1:A:284:PRO:O	1:A:287:GLN:HG2	2.07	0.55
1:A:157:ARG:HB3	1:A:161:HIS:HB3	1.89	0.55
1:A:175:LEU:HB3	1:A:233:MET:HG2	1.90	0.54
1:A:35:ILE:HG22	1:A:39:THR:O	2.08	0.53
1:A:1:MET:SD	1:A:2:GLU:N	2.82	0.52
1:A:174:LEU:HB3	1:A:212:LEU:HD13	1.91	0.52
1:A:124:LEU:HD22	1:A:150:ARG:NE	2.26	0.51
1:A:112:LEU:HB3	1:A:281:LEU:HD13	1.92	0.51
1:A:11:GLY:O	1:A:18:VAL:HG13	2.10	0.51
1:A:164:VAL:O	1:A:165:THR:HB	2.11	0.50
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.94	0.49
1:A:52:ILE:HA	1:A:55:LEU:HD22	1.94	0.49
1:A:287:GLN:HG3	1:A:288:ASP:N	2.20	0.48
1:A:31:ALA:CB	2:A:300:D05:H12	2.44	0.48
1:A:108:LEU:HD13	1:A:286:PHE:HZ	1.79	0.48
1:A:117:PHE:O	1:A:121:HIS:HD2	1.97	0.47
1:A:159:TYR:HD1	1:A:161:HIS:HE1	1.62	0.47
1:A:5:GLN:HG3	1:A:24:LYS:HD2	1.96	0.46
1:A:46:SER:O	1:A:50:ARG:HG3	2.16	0.46
1:A:143:LEU:HD13	1:A:146:PHE:HE1	1.80	0.46
1:A:49:ILE:HA	1:A:52:ILE:HG22	1.97	0.46
1:A:96:LEU:H	1:A:96:LEU:HD12	1.79	0.45
1:A:270:ASP:HA	1:A:271:PRO:HD3	1.71	0.45
1:A:64:VAL:HG13	1:A:143:LEU:O	2.17	0.45
1:A:35:ILE:O	1:A:40:GLU:HB2	2.17	0.45
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.31	0.45
1:A:75:LYS:HB2	1:A:77:TYR:CE2	2.51	0.45
1:A:252:VAL:O	1:A:252:VAL:HG23	2.17	0.45
1:A:169:ARG:HH21	1:A:170:ALA:H	1.66	0.44
1:A:10:ILE:CD1	1:A:82:PHE:HE1	2.30	0.44
1:A:156:VAL:HG11	3:A:387:HOH:O	2.18	0.44
1:A:124:LEU:HD22	1:A:150:ARG:CZ	2.47	0.44
1:A:173:ILE:HG12	1:A:180:TYR:CD2	2.53	0.44
1:A:177:CYS:HA	1:A:178:LYS:HD3	2.00	0.44
1:A:152:PHE:HA	3:A:384:HOH:O	2.18	0.44
1:A:183:ALA:HB1	1:A:274:ARG:HD2	2.00	0.43
1:A:253:PRO:HA	1:A:254:PRO:HA	1.79	0.43
1:A:175:LEU:HB3	1:A:233:MET:CG	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HD2	1:A:89:LYS:HA	1.80	0.42
1:A:168:TYR:CE1	1:A:192:ILE:HD13	2.54	0.42
1:A:189:LEU:HA	1:A:189:LEU:HD23	1.87	0.42
1:A:15:TYR:CE2	1:A:152:PHE:HB2	2.55	0.42
1:A:84:HIS:O	2:A:300:D05:H26	2.20	0.41
1:A:129:LYS:HG2	1:A:132:ASN:ND2	2.32	0.41
1:A:41:THR:HB	1:A:42:GLU:HA	2.02	0.41
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.77	0.41
1:A:38:ASP:HA	1:A:39:THR:HA	1.82	0.41
1:A:154:VAL:HA	1:A:155:PRO:HD3	1.86	0.41
1:A:248:PHE:CE2	1:A:263:LEU:HD13	2.56	0.41
1:A:105:LYS:HG2	1:A:289:VAL:HG13	2.02	0.41
1:A:210:ASP:O	1:A:214:ARG:HG3	2.20	0.40
1:A:9:LYS:HA	1:A:19:TYR:CD2	2.56	0.40
1:A:10:ILE:CG1	1:A:18:VAL:HG22	2.51	0.40
1:A:223:ASP:OD1	1:A:225:VAL:HG22	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:HE21	3:A:339:HOH:H1[3_848]	1.17	0.43
1:A:23:ASN:HD22	1:A:179:TYR:OH[4_529]	1.44	0.16

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	296/298 (99%)	268 (90%)	20 (7%)	8 (3%)	4 0

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	THR
1	A	160	THR
1	A	164	VAL
1	A	126	ARG
1	A	149	ALA
1	A	150	ARG
1	A	15	TYR
1	A	58	LEU

5.3.2 Protein sidechains [i](#)

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	263/263 (100%)	195 (74%)	68 (26%)	0 0

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	10	ILE
1	A	17	VAL
1	A	18	VAL
1	A	25	LEU
1	A	29	VAL
1	A	32	LEU
1	A	33	LYS
1	A	36	ARG
1	A	37	LEU
1	A	38	ASP
1	A	42	GLU
1	A	44	VAL
1	A	49	ILE
1	A	52	ILE
1	A	55	LEU
1	A	56	LYS
1	A	58	LEU
1	A	64	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	66	LEU
1	A	69	VAL
1	A	72	THR
1	A	73	GLU
1	A	77	TYR
1	A	79	VAL
1	A	83	LEU
1	A	96	LEU
1	A	101	LEU
1	A	103	LEU
1	A	108	LEU
1	A	111	LEU
1	A	112	LEU
1	A	123	VAL
1	A	124	LEU
1	A	126	ARG
1	A	128	LEU
1	A	131	GLN
1	A	132	ASN
1	A	134	LEU
1	A	138	GLU
1	A	148	LEU
1	A	150	ARG
1	A	158	THR
1	A	160	THR
1	A	163	VAL
1	A	164	VAL
1	A	165	THR
1	A	166	LEU
1	A	174	LEU
1	A	175	LEU
1	A	178	LYS
1	A	184	VAL
1	A	189	LEU
1	A	197	VAL
1	A	200	ARG
1	A	212	LEU
1	A	219	LEU
1	A	225	VAL
1	A	230	VAL
1	A	249	SER
1	A	251	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	SER
1	A	262	LEU
1	A	263	LEU
1	A	281	LEU
1	A	289	VAL
1	A	293	VAL
1	A	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	119	HIS
1	A	121	HIS
1	A	125	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
2	D05	A	300	-	31,33,33	1.43	6 (19%)	41,49,49	2.59	15 (36%)

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
2	D05	A	300	-	-	0/9/10/10	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	D05	C22-C23	2.86	1.43	1.38
2	A	300	D05	C20-C7	2.61	1.53	1.49
2	A	300	D05	C4-C9	-2.40	1.39	1.44
2	A	300	D05	C14-CL14	2.26	1.79	1.74
2	A	300	D05	C15-C16	2.17	1.42	1.38
2	A	300	D05	C5-N1	2.04	1.39	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	D05	C9-N8-C7	-8.45	119.02	123.90
2	A	300	D05	C12-C11-N1	6.66	126.05	120.55
2	A	300	D05	C4-C5-N6	-5.34	121.40	127.53
2	A	300	D05	C11-N1-N2	4.13	125.00	119.07
2	A	300	D05	C13-C14-C15	-3.87	116.94	121.64
2	A	300	D05	C16-C11-N1	-3.38	117.76	120.55
2	A	300	D05	C15-C14-CL14	3.34	123.36	119.17
2	A	300	D05	C9-C4-C3	3.03	138.76	131.43
2	A	300	D05	C3-N2-N1	2.54	107.73	105.12
2	A	300	D05	O9-C9-C4	-2.30	118.77	125.69
2	A	300	D05	N1-C5-N6	2.25	129.20	125.90
2	A	300	D05	C12-C13-C14	2.20	121.20	118.72
2	A	300	D05	C13-C12-CL12	-2.16	114.91	118.45
2	A	300	D05	C16-C15-C14	2.15	121.15	118.72
2	A	300	D05	C11-C16-CL16	-2.11	116.86	120.22

There are no chirality outliers.

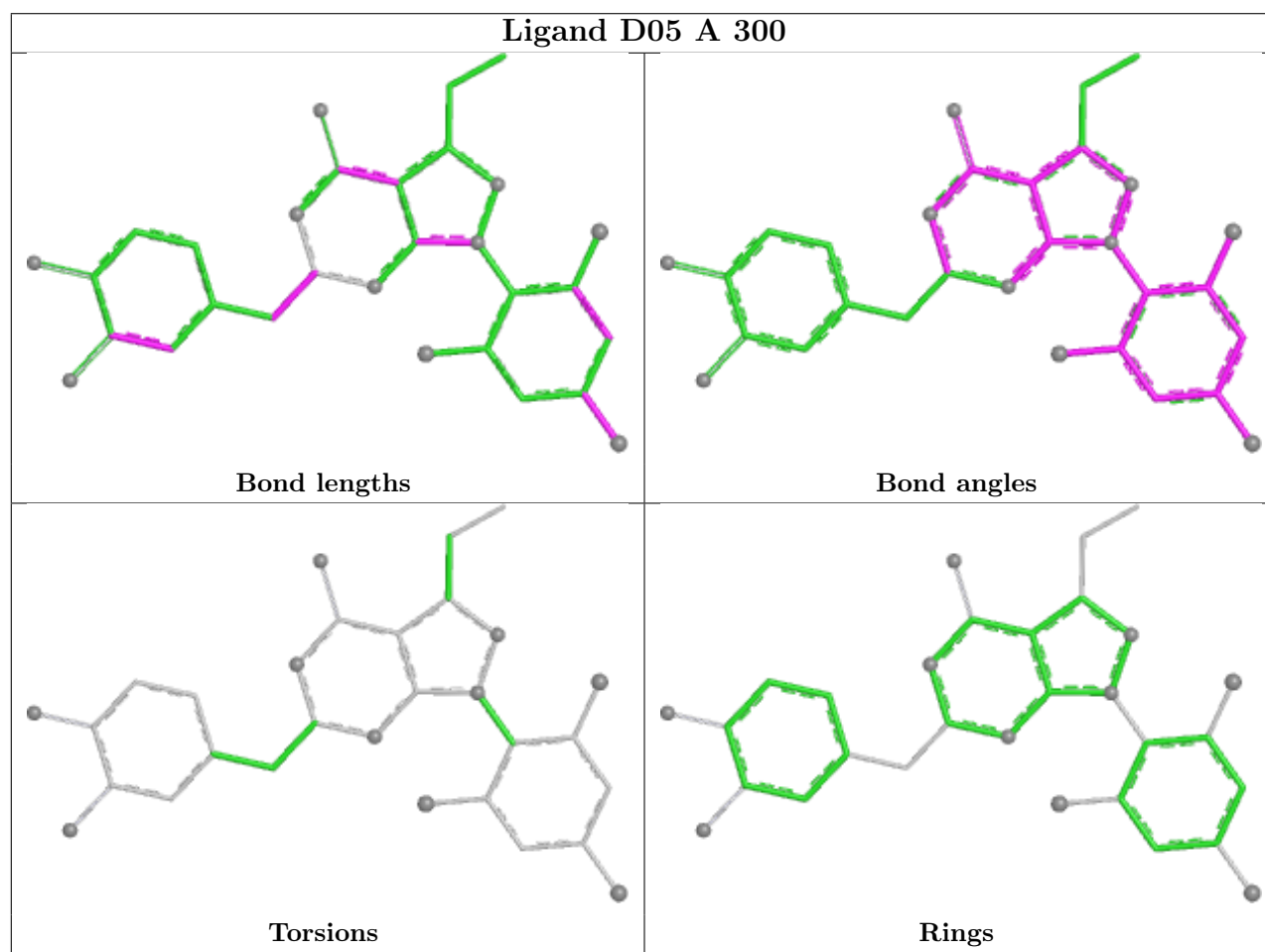
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	D05	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	298/298 (100%)	1.11	49 (16%) 4 4	13, 24, 64, 114	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	VAL	6.4
1	A	149	ALA	5.9
1	A	156	VAL	5.8
1	A	39	THR	5.6
1	A	298	LEU	5.3
1	A	41	THR	5.1
1	A	158	THR	5.0
1	A	164	VAL	4.4
1	A	37	LEU	4.3
1	A	40	GLU	4.1
1	A	296	LEU	4.0
1	A	159	TYR	3.9
1	A	163	VAL	3.9
1	A	297	ARG	3.8
1	A	155	PRO	3.6
1	A	295	HIS	3.6
1	A	25	LEU	3.5
1	A	1	MET	3.4
1	A	154	VAL	3.3
1	A	38	ASP	3.3
1	A	58	LEU	3.3
1	A	15	TYR	3.2
1	A	150	ARG	3.1
1	A	162	GLU	3.1
1	A	152	PHE	3.0
1	A	153	GLY	3.0
1	A	49	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	137	THR	2.9
1	A	42	GLU	2.9
1	A	14	THR	2.9
1	A	27	GLY	2.8
1	A	96	LEU	2.8
1	A	35	ILE	2.7
1	A	160	THR	2.6
1	A	43	GLY	2.6
1	A	151	ALA	2.6
1	A	52	ILE	2.4
1	A	2	GLU	2.4
1	A	248	PHE	2.4
1	A	47	THR	2.3
1	A	13	GLY	2.3
1	A	95	ALA	2.3
1	A	16	GLY	2.2
1	A	157	ARG	2.2
1	A	161	HIS	2.1
1	A	293	VAL	2.1
1	A	46	SER	2.0
1	A	11	GLY	2.0
1	A	10	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

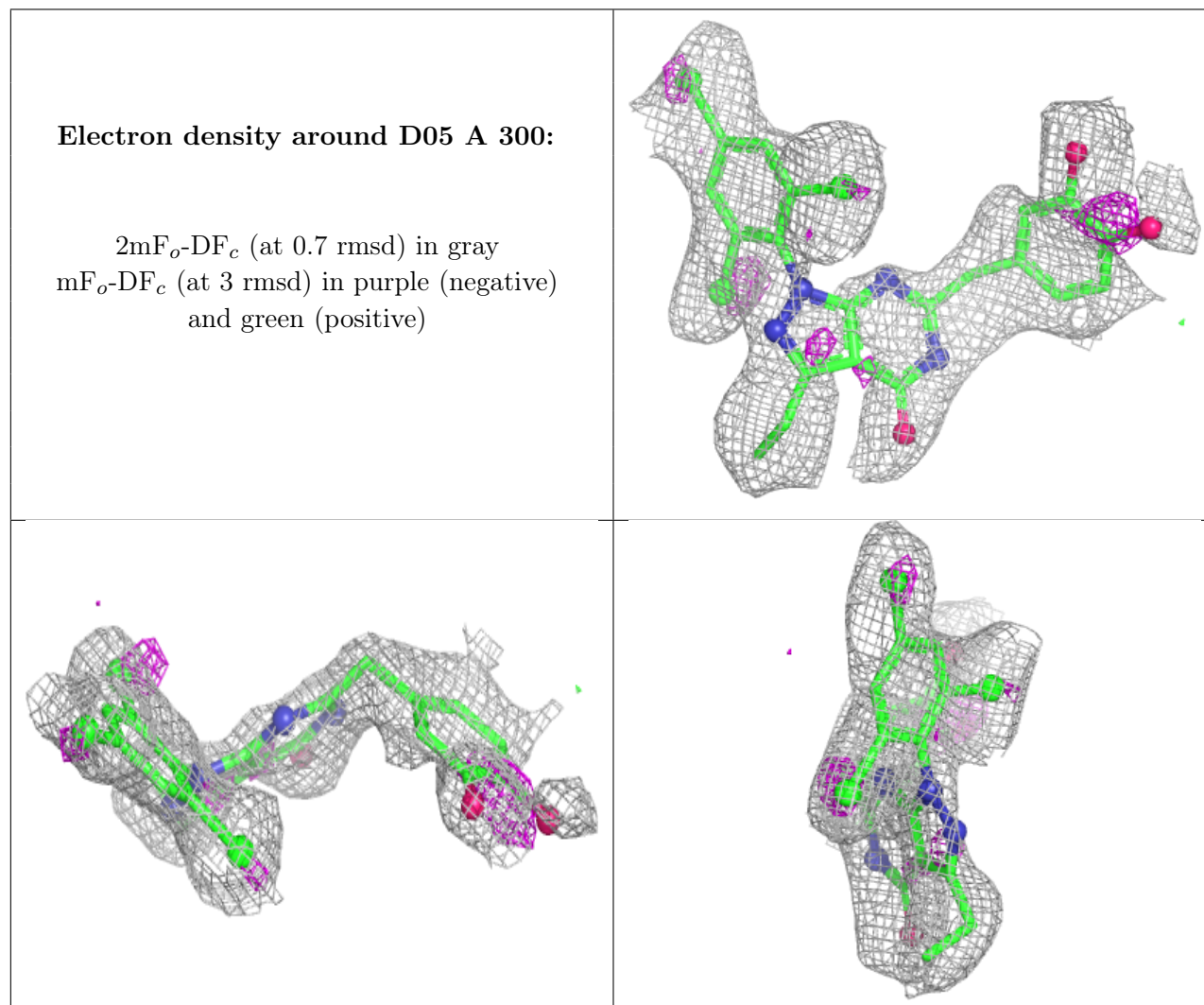
There are no oligosaccharides in this entry.

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
2	D05	A	300	30/30	0.82	0.12	26,34,38,39	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 ⓘ

There are no such residues in this entry.