



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:12 AM UTC

PDB ID : 7B7S / pdb_00007b7s
Title : CDK2/cyclin A2 in complex with 3H-pyrazolo[4,3-f]quinoline-based derivative HSD1368
Authors : Djukic, S.; Skerlova, J.; Rezacova, P.
Deposited on : 2020-12-11
Resolution : 2.54 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

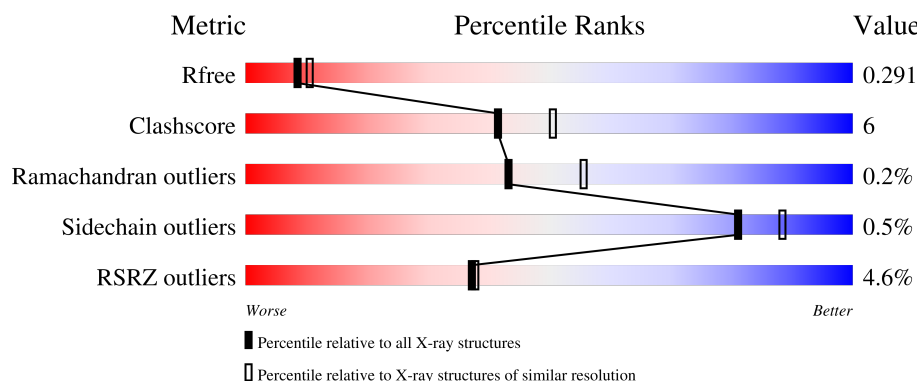
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	299	5% 80% 16% .
1	C	299	5% 82% 14% .
2	B	258	4% 79% 19% ..
2	D	258	3% 85% 12% ..

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
6	SGM	D	601	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8888 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	287	Total	C	N	O	P	S	0	1	0
			2318	1506	394	409	1	8			
1	C	288	Total	C	N	O	P	S	0	0	0
			2313	1503	393	408	1	8			

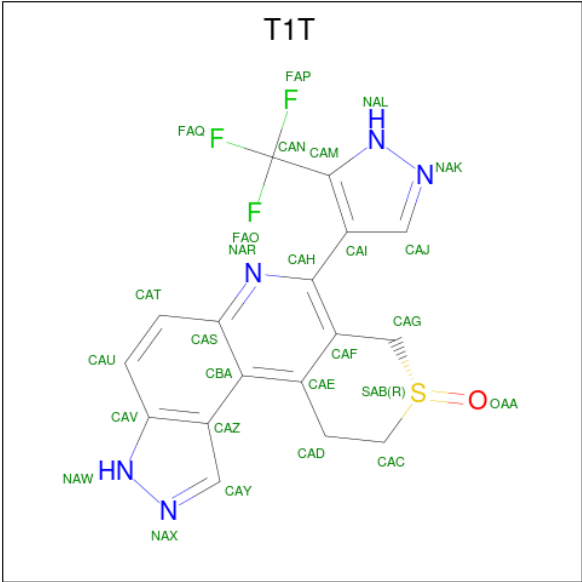
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

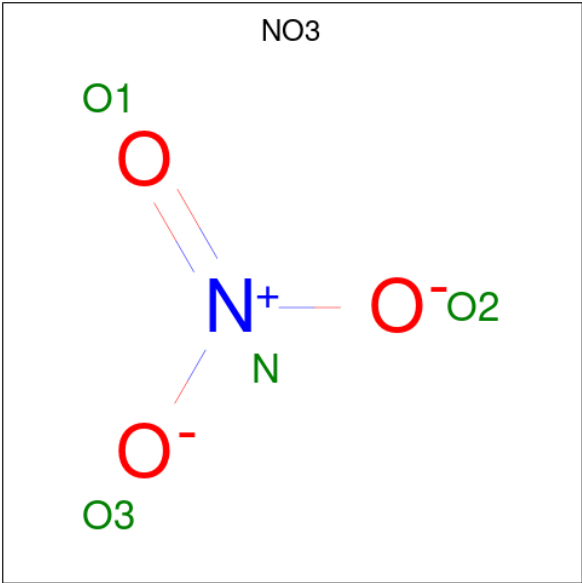
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	254	Total	C	N	O	S	0	0	0
			2053	1330	334	378	11			
2	D	254	Total	C	N	O	S	0	0	0
			2054	1330	334	379	11			

- Molecule 3 is 7-(3-(trifluoromethyl)-1H-pyrazol-4-yl)-3,8,10,11-tetrahydropyrazolo[4,3-f]thiopyrano[3,4-c]quinoline 9-oxide (CCD ID: T1T) (formula: C₁₇H₁₂F₃N₅OS) (labeled as "Ligand of Interest" by depositor).



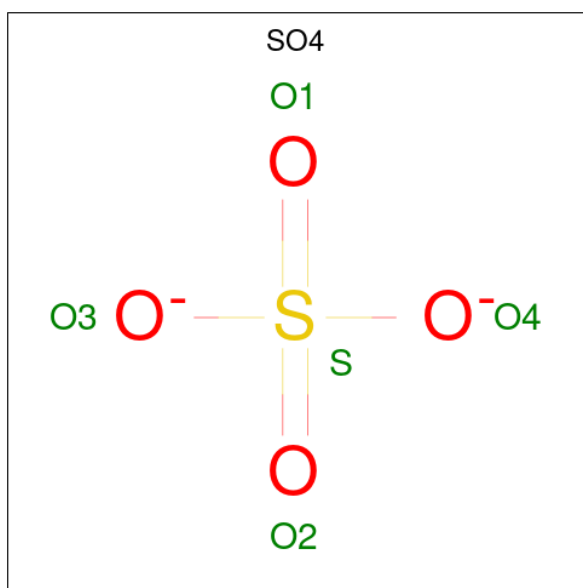
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	F	N	O	S	0	0
			27	17	3	5	1	1		
3	C	1	Total	C	F	N	O	S	0	0
			27	17	3	5	1	1		

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



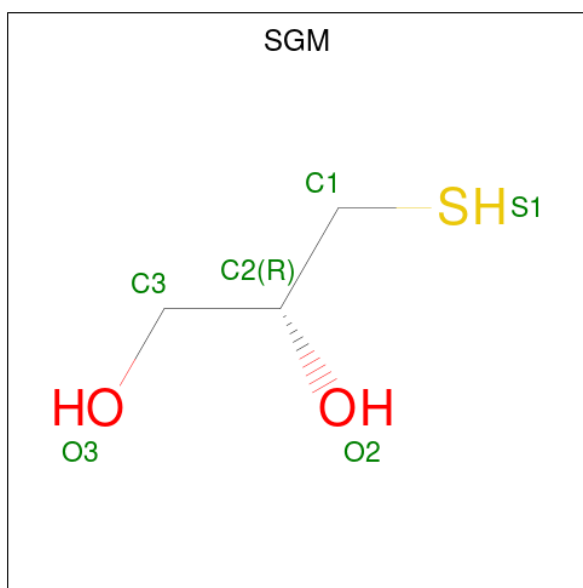
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	N O	0	0
			4	1 3		
4	C	1	Total	N O	0	0
			4	1 3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is MONOTHIOGLYCEROL (CCD ID: SGM) (formula: C₃H₈O₂S).



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

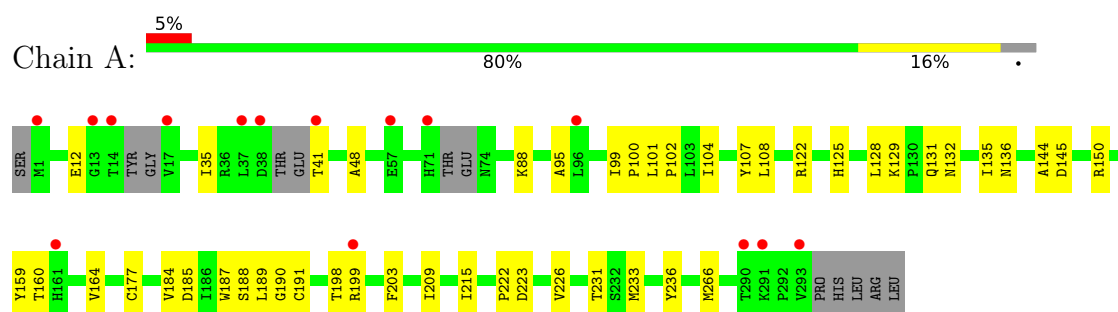
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total 17	O 17	0	0
7	B	20	Total 20	O 20	0	0
7	C	26	Total 26	O 26	0	0
7	D	14	Total 14	O 14	0	0

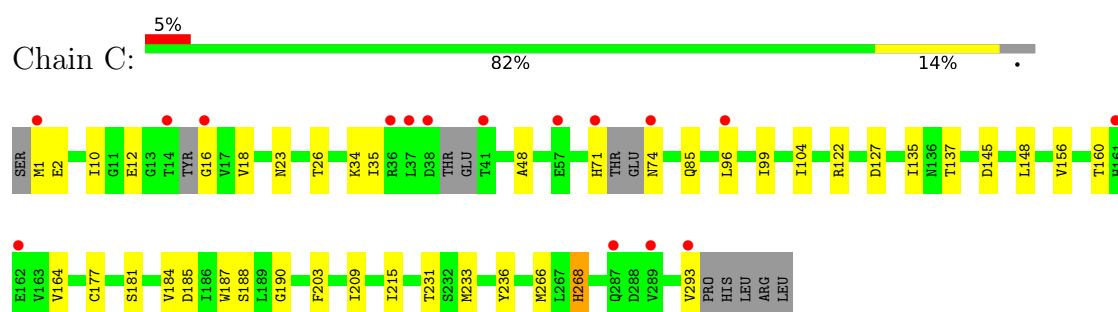
3 Residue-property plots [i](#)

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.

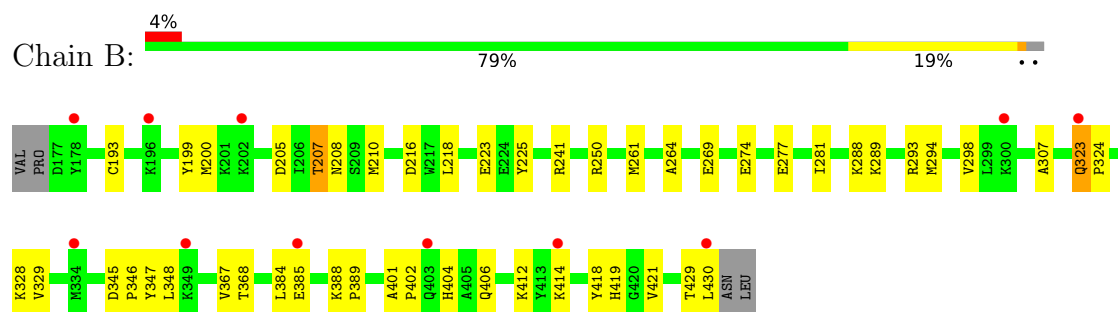
• Molecule 1: Cyclin-dependent kinase 2



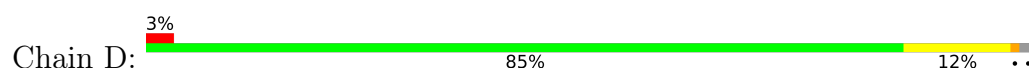
• Molecule 1: Cyclin-dependent kinase 2

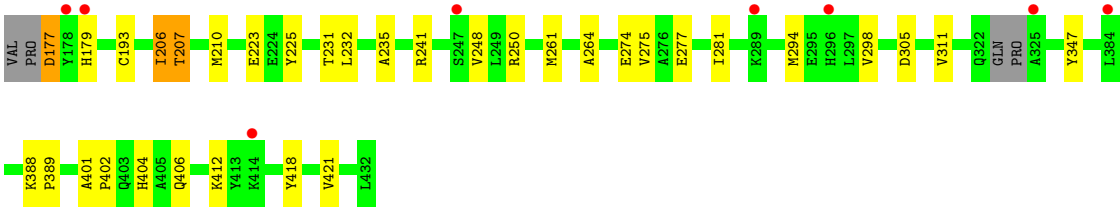


• Molecule 2: Cyclin-A2



• Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.08Å 164.70Å 73.41Å 90.00° 106.28° 90.00°	Depositor
Resolution (Å)	47.10 – 2.54 47.10 – 2.54	Depositor EDS
% Data completeness (in resolution range)	84.1 (47.10-2.54) 84.1 (47.10-2.54)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.246 , 0.291 0.249 , 0.291	Depositor DCC
R_{free} test set	2129 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8888	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.78% 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: SO4, NO3, SGM, T1T, 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	1.18	3/2362 (0.1%)	1.45	4/3198 (0.1%)
1	C	1.17	1/2357 (0.0%)	1.45	5/3191 (0.2%)
2	B	1.17	1/2102 (0.0%)	1.55	5/2853 (0.2%)
2	D	1.14	1/2101 (0.0%)	1.53	4/2848 (0.1%)
All	All	1.16	6/8922 (0.1%)	1.49	18/12090 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	PRO	C-O	-6.00	1.16	1.23
1	A	125	HIS	C-O	5.85	1.30	1.24
2	B	216	ASP	C-O	5.30	1.30	1.24
2	D	311	VAL	C-O	5.19	1.30	1.24
1	C	268	HIS	CE1-NE2	5.17	1.37	1.32
1	A	191	CYS	C-O	5.12	1.30	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	185	ASP	CA-CB-CG	6.22	118.82	112.60
1	C	184	VAL	O-C-N	6.15	128.08	121.87
2	D	177	ASP	CA-CB-CG	5.93	118.53	112.60
2	D	275	VAL	N-CA-C	-5.79	105.09	110.53
2	D	347	TYR	CB-CA-C	5.75	120.33	110.79
2	B	264	ALA	N-CA-C	-5.48	105.40	111.71
2	B	269	GLU	CA-C-O	-5.47	114.91	120.71
2	D	264	ALA	N-CA-C	-5.43	105.46	111.71
2	B	323	GLN	N-CA-C	-5.33	105.51	112.75
1	A	184	VAL	O-C-N	5.32	127.24	121.87
1	C	12	GLU	CB-CA-C	-5.29	100.81	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	LYS	CA-C-O	-5.26	115.28	120.70
2	B	414	LYS	N-CA-C	-5.24	107.02	113.41
1	A	185	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	12	GLU	CB-CA-C	-5.15	100.59	109.86
2	B	347	TYR	CB-CA-C	5.13	119.56	110.85
1	C	96	LEU	CA-C-N	5.01	127.00	120.28
1	C	96	LEU	C-N-CA	5.01	127.00	120.28

There are no chirality outliers.

There are no planarity outliers.

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	2318	0	2366	30	0
1	C	2313	0	2362	26	0
2	B	2053	0	2074	34	0
2	D	2054	0	2075	24	0
3	A	27	0	0	2	0
3	C	27	0	0	6	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
5	A	5	0	0	0	0
6	D	6	0	8	5	0
7	A	17	0	0	0	0
7	B	20	0	0	0	0
7	C	26	0	0	0	0
7	D	14	0	0	0	0
All	All	8888	0	8885	113	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 6.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:CYS:SG	6:D:601:SGM:S1	2.34	1.21
1:C:85:GLN:HG2	1:C:135:ILE:HD11	1.64	0.78
1:C:10:ILE:CG2	3:C:301:T1T:CAC	2.64	0.76
2:B:323:GLN:HB2	2:B:324:PRO:HD3	1.72	0.71
2:D:206:ILE:HD12	2:D:248:VAL:O	1.90	0.71
1:C:10:ILE:HG21	3:C:301:T1T:CAC	2.22	0.69
2:B:289:LYS:HG3	2:B:293:ARG:HD3	1.76	0.66
1:C:85:GLN:HB3	1:C:135:ILE:HG13	1.80	0.64
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.80	0.63
2:D:231:THR:HG22	2:D:261:MET:HE2	1.80	0.62
1:C:18:VAL:HG21	3:C:301:T1T:FAQ	1.92	0.60
2:B:274:GLU:HG2	2:B:277:GLU:HG3	1.84	0.59
1:C:1:MET:HE3	1:C:2:GLU:HB2	1.83	0.59
2:B:367:VAL:HG23	2:B:368:THR:HG23	1.83	0.59
2:D:210:MET:HE1	2:D:250:ARG:HD3	1.85	0.57
2:B:205:ASP:OD1	2:B:250:ARG:NH2	2.38	0.56
1:C:35:ILE:HD13	1:C:48:ALA:HB2	1.87	0.56
2:B:429:THR:C	2:B:430:LEU:HD12	2.30	0.56
1:A:35:ILE:HD13	1:A:48:ALA:HB2	1.87	0.56
2:D:305:ASP:HB3	6:D:601:SGM:H31	1.88	0.56
1:C:10:ILE:HG22	3:C:301:T1T:CAC	2.37	0.55
3:A:301:T1T:CAY	3:A:301:T1T:CAD	2.85	0.54
1:A:95:ALA:O	1:A:199:ARG:HD2	2.08	0.54
1:A:99:ILE:HG22	1:A:104:ILE:HG13	1.90	0.54
1:A:198:THR:C	1:A:199:ARG:HG2	2.33	0.53
1:C:127:ASP:OD2	1:C:148:LEU:HD12	2.07	0.53
2:B:218:LEU:HB3	2:B:261:MET:CE	2.38	0.53
2:B:218:LEU:HB3	2:B:261:MET:HE2	1.91	0.53
2:B:329:VAL:HG23	2:B:367:VAL:HG21	1.90	0.52
1:C:145:ASP:HB2	3:C:301:T1T:CAJ	2.39	0.52
2:B:328:LYS:HE2	2:B:419:HIS:HB3	1.93	0.51
1:C:99:ILE:HG22	1:C:104:ILE:HG13	1.93	0.51
1:C:16:GLY:N	1:C:34:LYS:O	2.44	0.51
1:A:131[B]:GLN:O	1:A:131[B]:GLN:HG3	2.10	0.51
1:A:129:LYS:HE3	1:A:131[B]:GLN:HG2	1.92	0.50
1:A:223:ASP:H	1:A:226:VAL:HG22	1.77	0.50
1:A:222:PRO:HA	1:A:226:VAL:HG21	1.93	0.50
2:B:210:MET:HE1	2:B:250:ARG:HH11	1.75	0.49
2:B:223:GLU:OE2	2:B:412:LYS:HE3	2.12	0.49
2:D:223:GLU:OE2	2:D:412:LYS:HE3	2.12	0.49
1:A:101:LEU:HB2	1:A:102:PRO:CD	2.43	0.49
1:A:231:THR:HA	1:A:236:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD12	1:C:18:VAL:HG12	1.94	0.49
2:B:207:THR:HG22	2:B:210:MET:SD	2.53	0.49
2:B:329:VAL:CG2	2:B:367:VAL:CG2	2.90	0.49
1:C:71:HIS:NE2	1:C:74:ASN:HA	2.29	0.48
1:A:122:ARG:HH21	2:B:307:ALA:HB1	1.79	0.48
1:C:137:THR:O	1:C:293:VAL:HG13	2.14	0.48
2:D:206:ILE:CD1	2:D:248:VAL:O	2.60	0.48
2:B:385:GLU:HA	2:B:388:LYS:HE3	1.94	0.48
1:C:177:CYS:HB2	1:C:233:MET:CE	2.42	0.48
2:D:210:MET:CE	2:D:250:ARG:HD3	2.43	0.48
2:D:210:MET:SD	2:D:250:ARG:HG2	2.53	0.48
2:B:388:LYS:HB2	2:B:389:PRO:HD3	1.96	0.47
1:A:41:THR:O	2:B:288:LYS:NZ	2.36	0.47
1:A:198:THR:O	1:A:199:ARG:HG2	2.15	0.47
1:A:128:LEU:HD13	1:A:189:LEU:CD1	2.45	0.47
2:B:429:THR:O	2:B:430:LEU:HD12	2.14	0.47
2:D:401:ALA:N	2:D:402:PRO:CD	2.78	0.47
2:D:404:HIS:CE1	2:D:406:GLN:OE1	2.68	0.47
2:D:177:ASP:HB2	2:D:179:HIS:CE1	2.50	0.46
1:A:159:TYR:O	1:A:160:TPO:C	2.64	0.46
2:B:401:ALA:N	2:B:402:PRO:CD	2.78	0.46
1:C:231:THR:HA	1:C:236:TYR:CD1	2.51	0.46
1:C:156:VAL:HG21	1:C:181:SER:HB2	1.98	0.46
2:B:404:HIS:CE1	2:B:406:GLN:OE1	2.68	0.46
2:D:274:GLU:HG2	2:D:277:GLU:HG3	1.98	0.46
2:B:329:VAL:HG22	2:B:367:VAL:CG2	2.46	0.46
2:D:225:TYR:HE2	2:D:281:ILE:HG21	1.81	0.46
2:B:329:VAL:HG22	2:B:367:VAL:HG22	1.97	0.45
2:D:235:ALA:HB2	2:D:261:MET:HE3	1.98	0.45
1:C:85:GLN:HG2	1:C:135:ILE:CD1	2.39	0.45
2:D:207:THR:CG2	2:D:210:MET:HG3	2.46	0.45
2:B:193:CYS:O	2:B:241:ARG:HD2	2.17	0.45
2:B:345:ASP:HA	2:B:346:PRO:HA	1.73	0.44
2:D:305:ASP:CG	6:D:601:SGM:H31	2.42	0.44
1:A:101:LEU:HB2	1:A:102:PRO:HD3	1.98	0.44
1:A:190:GLY:N	1:A:266:MET:HE2	2.33	0.44
1:C:190:GLY:N	1:C:266:MET:HE2	2.33	0.44
2:B:329:VAL:CG2	2:B:367:VAL:HG21	2.48	0.43
2:B:225:TYR:HE2	2:B:281:ILE:HG21	1.84	0.43
2:B:384:LEU:HD23	2:B:384:LEU:HA	1.88	0.43
2:D:294:MET:O	2:D:298:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:HB2	3:A:301:T1T:CAJ	2.49	0.43
2:D:305:ASP:CB	6:D:601:SGM:H31	2.49	0.43
2:B:294:MET:O	2:B:298:VAL:HG23	2.18	0.43
2:B:418:TYR:O	2:B:421:VAL:HG13	2.20	0.42
1:A:177:CYS:HB2	1:A:233:MET:CE	2.49	0.42
1:A:107:TYR:O	1:A:108:LEU:C	2.63	0.42
1:C:203:PHE:CE1	1:C:215:ILE:HA	2.55	0.42
2:D:418:TYR:O	2:D:421:VAL:HG13	2.19	0.42
1:C:122:ARG:O	1:C:122:ARG:HG3	2.20	0.42
2:D:193:CYS:O	2:D:241:ARG:HD2	2.20	0.42
2:D:232:LEU:HA	2:D:261:MET:HE1	2.01	0.42
2:D:305:ASP:HB3	6:D:601:SGM:C3	2.50	0.42
1:C:23:ASN:HB3	1:C:26:THR:OG1	2.20	0.42
1:A:187:TRP:O	1:A:188:SER:C	2.63	0.41
1:A:203:PHE:CE1	1:A:215:ILE:HA	2.55	0.41
1:A:209:ILE:HD12	1:A:209:ILE:HA	1.91	0.41
2:B:200:MET:HG2	2:B:208:ASN:OD1	2.20	0.41
2:B:274:GLU:CG	2:B:277:GLU:HG3	2.51	0.41
1:A:177:CYS:HB2	1:A:233:MET:HE1	2.01	0.41
1:C:18:VAL:CG2	3:C:301:T1T:FAQ	2.57	0.41
1:A:122:ARG:O	1:A:122:ARG:HG3	2.20	0.41
1:A:128:LEU:HD13	1:A:189:LEU:HD13	2.00	0.41
1:C:187:TRP:O	1:C:188:SER:C	2.62	0.41
1:C:209:ILE:HD12	1:C:209:ILE:HA	1.95	0.41
1:A:101:LEU:CB	1:A:102:PRO:CD	2.99	0.41
2:B:207:THR:HG23	2:B:210:MET:H	1.85	0.41
1:A:135:ILE:HG22	1:A:136:ASN:O	2.21	0.40
2:B:199:TYR:HE2	2:B:348:LEU:HD11	1.85	0.40
1:A:132:ASN:O	1:A:144:ALA:HB3	2.22	0.40
1:A:223:ASP:O	1:A:226:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/299 (93%)	265 (95%)	13 (5%)	1 (0%)	30	39
1	C	279/299 (93%)	263 (94%)	15 (5%)	1 (0%)	30	39
2	B	252/258 (98%)	242 (96%)	10 (4%)	0	100	100
2	D	250/258 (97%)	240 (96%)	10 (4%)	0	100	100
All	All	1060/1114 (95%)	1010 (95%)	48 (4%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL

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	253/263 (96%)	252 (100%)	1 (0%)	84	90
1	C	252/263 (96%)	251 (100%)	1 (0%)	84	90
2	B	228/232 (98%)	227 (100%)	1 (0%)	84	90
2	D	228/232 (98%)	226 (99%)	2 (1%)	70	82
All	All	961/990 (97%)	956 (100%)	5 (0%)	81	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
2	B	207	THR
1	C	268	HIS
2	D	206	ILE
2	D	207	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
2	B	396	GLN
2	B	403	GLN
1	C	5	GLN
1	C	85	GLN
1	C	268	HIS
2	D	179	HIS
2	D	183	HIS

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	1.18	1 (12%)	10,14,16	1.05	0
1	TPO	A	160	1	8,10,11	0.60	0	10,14,16	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O1P	2.62	1.58	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	CB-OG1-P-O2P
1	A	160	TPO	CB-OG1-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	NO3	A	302	-	1,3,3	0.41	0	0,3,3	-	-
3	T1T	C	301	-	30,31,31	3.97	16 (53%)	35,48,48	2.50	13 (37%)
5	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.15	0
3	T1T	A	301	-	30,31,31	4.64	17 (56%)	35,48,48	2.55	16 (45%)
4	NO3	C	302	-	1,3,3	0.38	0	0,3,3	-	-
6	SGM	D	601	-	5,5,5	0.33	0	5,5,5	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	T1T	A	301	-	-	6/10/19/19	0/4/5/5
6	SGM	D	601	-	-	0/4/4/4	-
3	T1T	C	301	-	-	8/10/19/19	0/4/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	T1T	CAH-CAI	-12.44	1.34	1.49
3	A	301	T1T	CAH-CAI	-12.24	1.34	1.49
3	A	301	T1T	CAZ-CAV	-9.18	1.32	1.41
3	C	301	T1T	CAC-SAB	8.07	1.96	1.80
3	A	301	T1T	CAC-SAB	7.63	1.95	1.80
3	A	301	T1T	NAW-NAX	-7.58	1.30	1.36
3	A	301	T1T	CAJ-CAI	-7.54	1.31	1.40
3	A	301	T1T	CAD-CAE	-7.43	1.38	1.51
3	A	301	T1T	CAZ-CAY	-7.41	1.33	1.42
3	C	301	T1T	CAZ-CAV	-6.92	1.34	1.41
3	C	301	T1T	CAJ-CAI	-5.91	1.33	1.40
3	C	301	T1T	NAW-NAX	-5.42	1.32	1.36
3	C	301	T1T	CAD-CAE	-5.30	1.42	1.51
3	A	301	T1T	CAU-CAV	-4.78	1.32	1.39
3	A	301	T1T	CAZ-CBA	-4.77	1.35	1.44
3	C	301	T1T	CAZ-CAY	-4.77	1.36	1.42
3	C	301	T1T	CAG-CAF	4.25	1.55	1.50
3	A	301	T1T	CAN-CAM	3.71	1.57	1.50
3	C	301	T1T	CAZ-CBA	-3.60	1.37	1.44
3	C	301	T1T	CAI-CAM	-3.57	1.34	1.38
3	A	301	T1T	CAH-CAF	-3.47	1.36	1.41
3	A	301	T1T	NAL-NAK	-3.21	1.31	1.36
3	C	301	T1T	CAU-CAV	-3.18	1.34	1.39
3	A	301	T1T	CAM-NAL	-3.15	1.31	1.34
3	A	301	T1T	CAE-CBA	-3.03	1.38	1.43
3	C	301	T1T	CAH-NAR	2.90	1.36	1.32
3	C	301	T1T	CAH-CAF	-2.36	1.37	1.41
3	A	301	T1T	CBA-CAS	-2.27	1.38	1.42
3	C	301	T1T	CAM-NAL	-2.26	1.32	1.34
3	C	301	T1T	NAL-NAK	-2.19	1.32	1.36
3	A	301	T1T	CAT-CAS	-2.16	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	T1T	CAT-CAS	-2.14	1.38	1.41
3	A	301	T1T	CAJ-NAK	-2.06	1.29	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	T1T	CAF-CAG-SAB	-8.05	94.35	114.14
3	A	301	T1T	CAH-CAF-CAE	5.73	123.00	118.99
3	A	301	T1T	CAF-CAG-SAB	-5.66	100.22	114.14
3	A	301	T1T	CAV-NAW-NAX	-5.24	108.95	111.52
3	C	301	T1T	CAF-CAH-CAI	-4.21	114.59	122.38
3	C	301	T1T	CAV-NAW-NAX	-4.18	109.47	111.52
3	A	301	T1T	CAF-CAH-NAR	-3.93	117.81	123.40
3	C	301	T1T	CAC-SAB-CAG	-3.77	90.80	97.50
3	A	301	T1T	CAH-CAI-CAJ	-3.59	113.63	125.09
3	C	301	T1T	CAH-CAF-CAE	3.57	121.49	118.99
3	A	301	T1T	CAJ-CAI-CAM	3.46	107.92	104.77
3	A	301	T1T	CAZ-CAY-NAX	-3.41	109.90	111.33
3	A	301	T1T	CAF-CAH-CAI	-3.35	116.19	122.38
3	C	301	T1T	CAF-CAH-NAR	-3.26	118.77	123.40
3	C	301	T1T	CAC-CAD-CAE	-3.23	109.00	113.64
3	A	301	T1T	CAU-CAV-CAZ	-2.87	120.39	122.66
3	A	301	T1T	CAZ-CAV-NAW	2.74	108.52	106.60
3	C	301	T1T	CBA-CAZ-CAY	2.72	135.54	125.79
3	C	301	T1T	CAZ-CAY-NAX	-2.46	110.29	111.33
3	C	301	T1T	CAH-CAI-CAJ	-2.46	117.23	125.09
3	C	301	T1T	CAM-NAL-NAK	-2.39	106.84	112.11
3	A	301	T1T	CAV-CAZ-CAY	2.30	105.79	104.41
3	C	301	T1T	CAJ-NAK-NAL	2.22	108.53	105.19
3	A	301	T1T	CAJ-NAK-NAL	2.20	108.50	105.19
3	C	301	T1T	CAU-CAT-CAS	-2.10	118.29	120.80
3	A	301	T1T	CBA-CAZ-CAY	2.09	133.27	125.79
3	A	301	T1T	CAC-CAD-CAE	-2.05	110.69	113.64
3	A	301	T1T	CAI-CAJ-NAK	-2.04	108.53	111.34
3	A	301	T1T	CAH-NAR-CAS	2.02	121.11	117.15

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	T1T	NAR-CAH-CAI-CAM
3	A	301	T1T	NAR-CAH-CAI-CAJ

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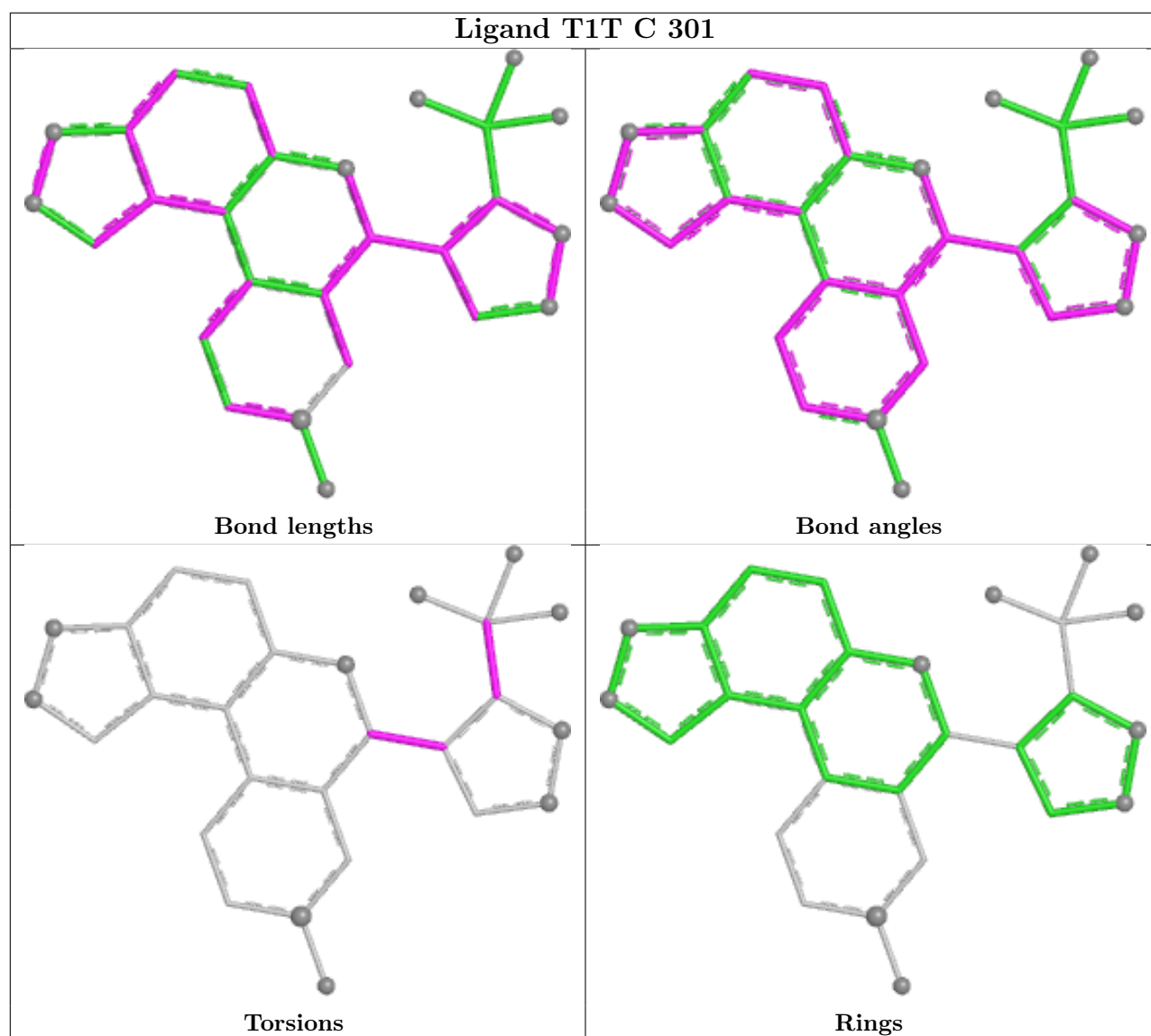
Mol	Chain	Res	Type	Atoms
3	C	301	T1T	NAR-CAH-CAI-CAM
3	C	301	T1T	NAR-CAH-CAI-CAJ
3	C	301	T1T	CAI-CAM-CAN-FAQ
3	C	301	T1T	CAI-CAM-CAN-FAO
3	C	301	T1T	CAI-CAM-CAN-FAP
3	A	301	T1T	CAF-CAH-CAI-CAJ
3	C	301	T1T	CAF-CAH-CAI-CAJ
3	A	301	T1T	NAL-CAM-CAN-FAO
3	A	301	T1T	NAL-CAM-CAN-FAP
3	A	301	T1T	NAL-CAM-CAN-FAQ
3	C	301	T1T	NAL-CAM-CAN-FAO
3	C	301	T1T	NAL-CAM-CAN-FAQ

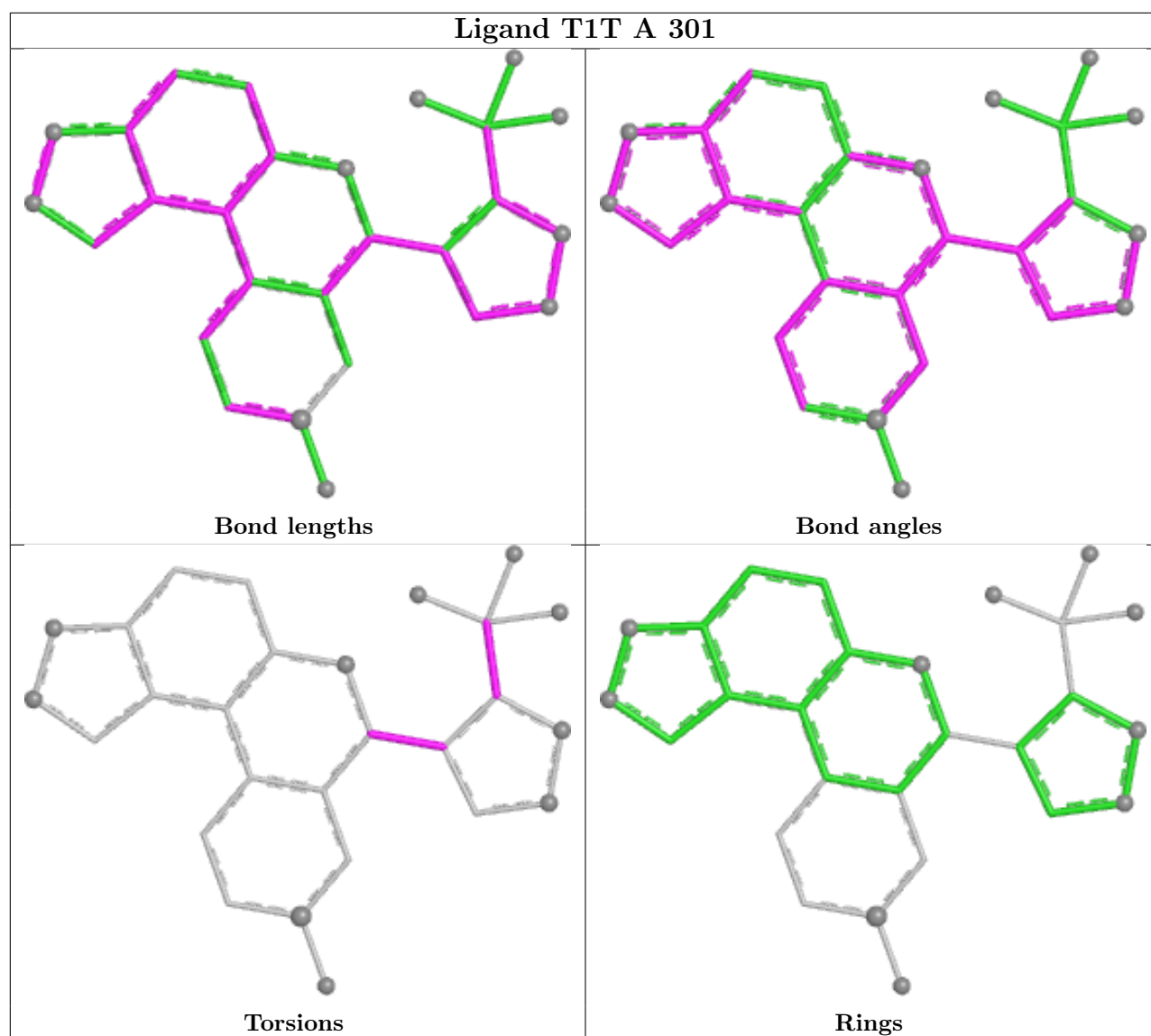
There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	T1T	6	0
3	A	301	T1T	2	0
6	D	601	SGM	5	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	286/299 (95%)	0.43	15 (5%)	33 32	15, 37, 69, 88	1 (0%)
1	C	287/299 (95%)	0.39	16 (5%)	30 29	21, 36, 66, 109	0
2	B	254/258 (98%)	0.37	11 (4%)	40 40	19, 35, 59, 91	0
2	D	254/258 (98%)	0.53	8 (3%)	51 52	21, 41, 61, 80	0
All	All	1081/1114 (97%)	0.43	50 (4%)	37 38	15, 37, 65, 109	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	THR	5.2
1	C	293	VAL	4.7
1	C	38	ASP	4.0
2	D	178	TYR	4.0
1	A	293	VAL	3.8
2	B	323	GLN	3.6
2	B	178	TYR	3.6
1	A	13	GLY	3.5
2	D	325	ALA	3.4
1	C	16	GLY	3.4
2	B	430	LEU	3.4
1	A	1	MET	3.2
1	A	291	LYS	3.2
1	A	57	GLU	3.1
1	C	1	MET	2.9
1	C	37	LEU	2.9
1	C	36	ARG	2.9
1	A	161	HIS	2.9
2	D	414	LYS	2.8
1	A	199	ARG	2.8
1	A	71	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	74	ASN	2.7
1	C	57	GLU	2.7
2	B	349	LYS	2.7
1	A	96	LEU	2.7
1	C	289	VAL	2.7
2	B	403	GLN	2.7
2	B	385	GLU	2.6
2	D	384	LEU	2.6
2	D	296	HIS	2.6
2	B	202	LYS	2.6
2	B	414	LYS	2.6
1	C	96	LEU	2.5
1	C	71	HIS	2.5
1	A	37	LEU	2.4
1	C	14	THR	2.4
2	D	247	SER	2.4
1	A	38	ASP	2.3
2	B	334	MET	2.3
1	C	41	THR	2.2
2	D	179	HIS	2.2
1	C	161	HIS	2.2
1	A	290	THR	2.2
2	D	289	LYS	2.2
1	A	41	THR	2.1
1	A	17	VAL	2.1
1	C	162	GLU	2.1
1	C	287	GLN	2.1
2	B	196	LYS	2.1
2	B	300	LYS	2.0

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

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	A	160	11/12	0.97	0.06	27,34,41,41	0
1	TPO	C	160	11/12	0.97	0.08	21,30,43,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

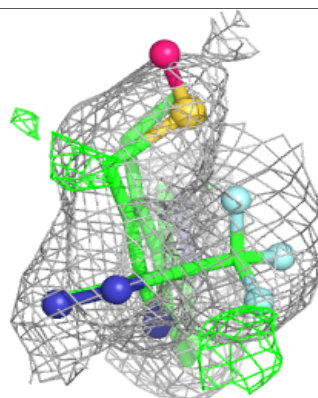
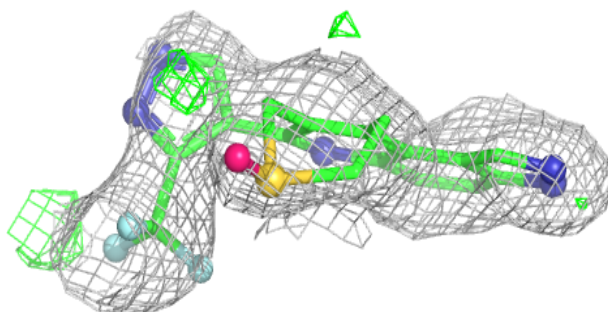
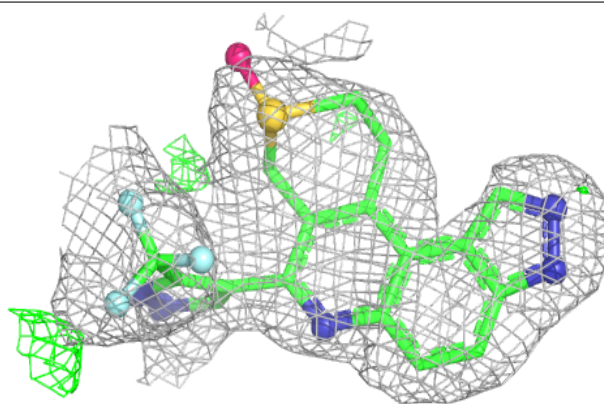
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	303	5/5	0.79	0.15	87,89,98,100	0
3	T1T	A	301	27/27	0.80	0.18	41,56,64,75	27
3	T1T	C	301	27/27	0.81	0.17	39,59,66,76	27
4	NO3	A	302	4/4	0.84	0.12	37,39,44,45	0
6	SGM	D	601	6/6	0.87	0.15	56,60,62,65	0
4	NO3	C	302	4/4	0.90	0.09	30,30,33,34	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.

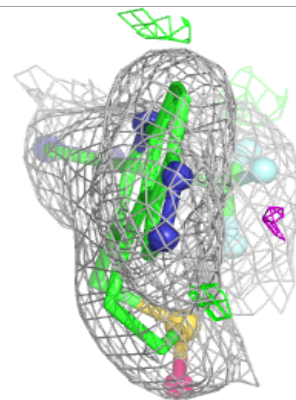
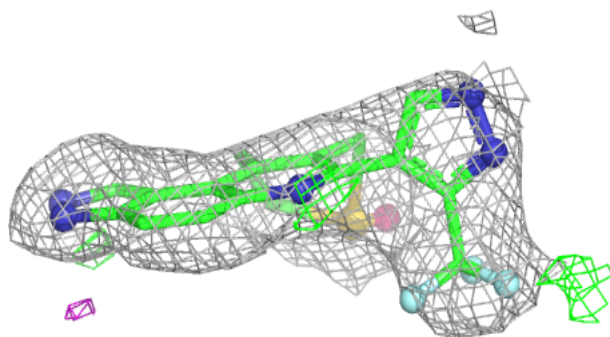
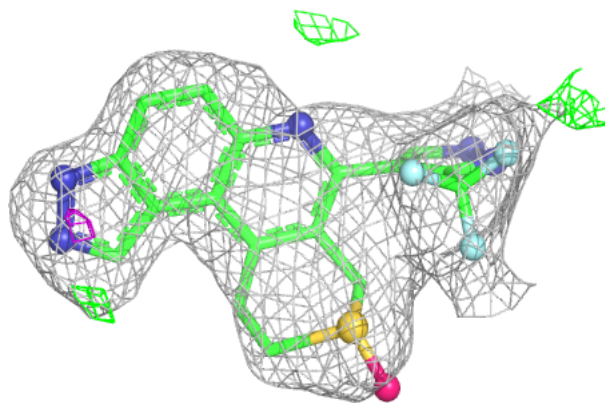
Electron density around T1T A 301:

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 T1T C 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.