



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:52 am BST

PDB ID : 4EOL
Title : Thr 160 phosphorylated CDK2 H84S, Q85M, K89D - human cyclin A3 complex with the inhibitor RO3306
Authors : Echalier, A.; Cot, E.; Camasses, A.; Hodimont, E.; Hoh, F.; Sheinerman, F.; Krasinska, L.; Fisher, D.
Deposited on : 2012-04-14
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

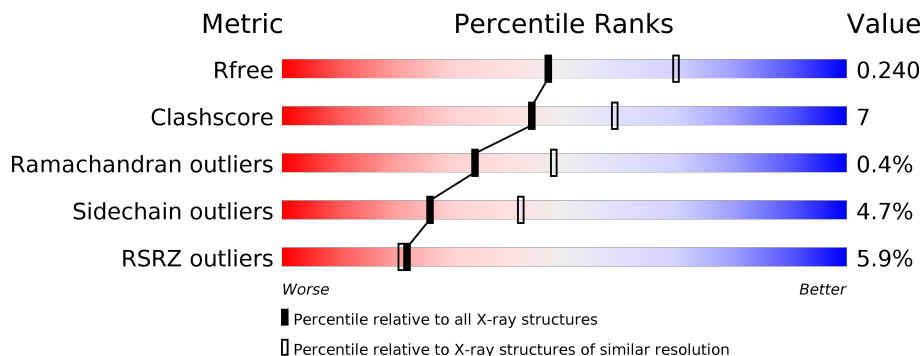
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	
1	C	300	
2	B	258	
2	D	258	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1RO	A	301	-	-	X	-
3	1RO	C	301	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9078 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	
			Total	C	N	O	P				S
1	A	295	Total	C	N	O	P	S	0	3	0
			2393	1551	405	427	1	9			
1	C	300	Total	C	N	O	P	S	0	1	0
			2414	1564	408	432	1	9			

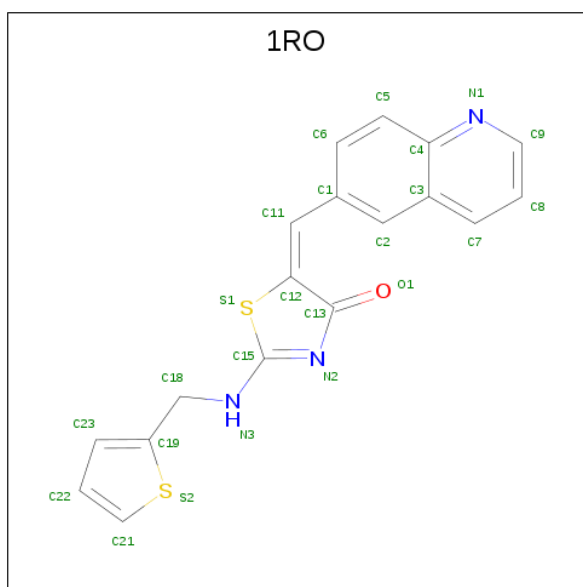
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	LEU	-	EXPRESSION TAG	UNP P24941
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	SER	-	EXPRESSION TAG	UNP P24941
A	84	SER	HIS	ENGINEERED MUTATION	UNP P24941
A	85	MET	GLN	ENGINEERED MUTATION	UNP P24941
A	89	ASP	LYS	ENGINEERED MUTATION	UNP P24941
C	-2	LEU	-	EXPRESSION TAG	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941
C	84	SER	HIS	ENGINEERED MUTATION	UNP P24941
C	85	MET	GLN	ENGINEERED MUTATION	UNP P24941
C	89	ASP	LYS	ENGINEERED MUTATION	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

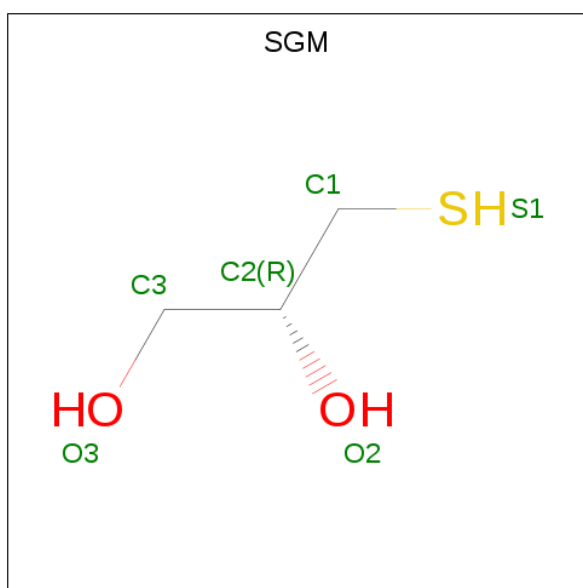
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	257	Total	C	N	O	S	0	0	0
			2076	1345	338	382	11			
2	D	256	Total	C	N	O	S	0	0	0
			2068	1339	337	381	11			

- Molecule 3 is (5E)-5-(quinolin-6-ylmethylidene)-2-[(thiophen-2-ylmethyl)amino]-1,3-thiazol-4(5H)-one (three-letter code: 1RO) (formula: C₁₈H₁₃N₃OS₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	18	3	1	2		
3	C	1	Total	C	N	O	S	0	0
			24	18	3	1	2		

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



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

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

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

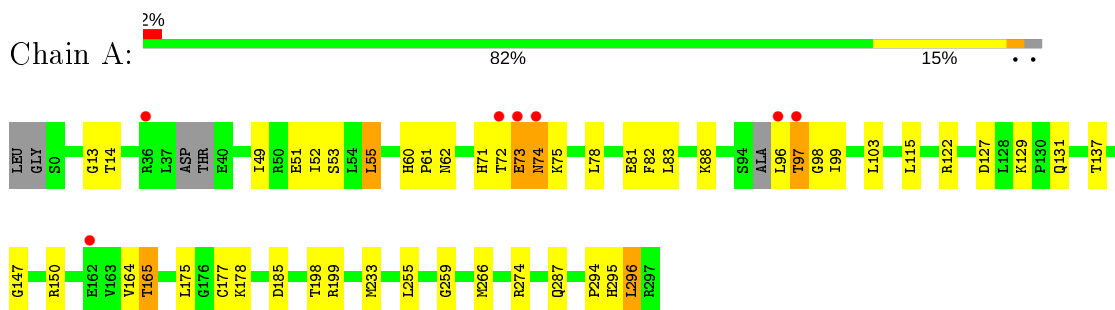
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total 36	O 36	0	0
6	B	14	Total 14	O 14	0	0
6	C	13	Total 13	O 13	0	0
6	D	3	Total 3	O 3	0	0

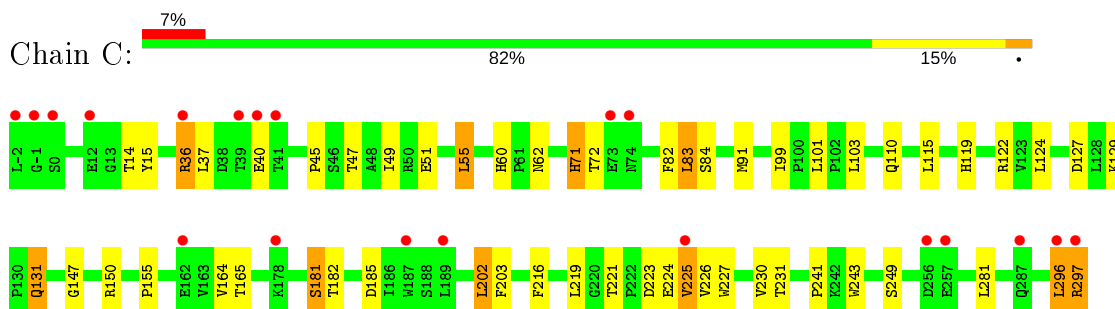
3 Residue-property plots [i](#)

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

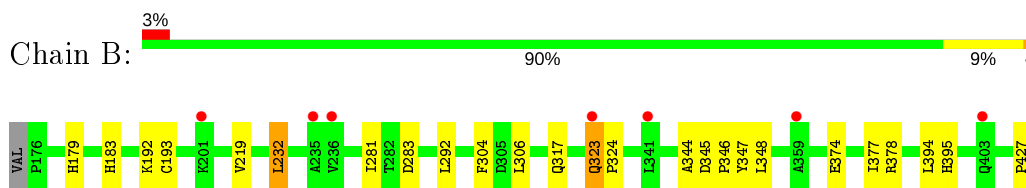
- Molecule 1: Cyclin-dependent kinase 2



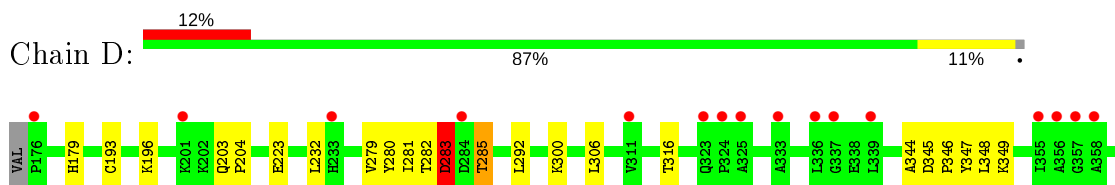
- Molecule 1: Cyclin-dependent kinase 2

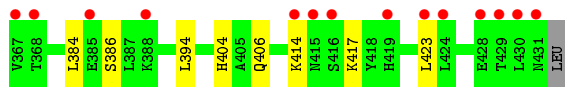


- Molecule 2: Cyclin-A2



- 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	73.85Å 133.94Å 173.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 28.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.40) 99.5 (28.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.246 0.217 , 0.240	Depositor DCC
R_{free} test set	3441 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9078	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: TPO, MG, SGM, 1RO

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	0.51	0/2440	0.61	3/3306 (0.1%)
1	C	0.54	0/2463	0.68	6/3341 (0.2%)
2	B	0.41	0/2126	0.52	0/2886
2	D	0.40	0/2118	0.51	0/2875
All	All	0.47	0/9147	0.59	9/12408 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	LEU	CB-CA-C	-12.39	86.66	110.20
1	C	297	ARG	N-CA-CB	9.38	127.49	110.60
1	C	181	SER	N-CA-C	9.28	136.05	111.00
1	C	182	THR	N-CA-CB	7.52	124.59	110.30
1	A	295	HIS	CB-CA-C	-6.20	98.00	110.40
1	C	84	SER	N-CA-CB	-5.64	102.04	110.50
1	A	296	LEU	N-CA-CB	-5.44	99.52	110.40
1	C	181	SER	CB-CA-C	-5.16	100.30	110.10
1	A	296	LEU	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2393	0	2421	40	0
1	C	2414	0	2454	42	0
2	B	2076	0	2098	13	0
2	D	2068	0	2087	18	0
3	A	24	0	13	10	0
3	C	24	0	13	7	0
4	B	6	0	7	2	0
4	D	6	0	7	3	0
5	B	1	0	0	0	0
6	A	36	0	0	0	0
6	B	14	0	0	0	0
6	C	13	0	0	0	0
6	D	3	0	0	0	0
All	All	9078	0	9100	119	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 7.

All (119) 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:124:LEU:CD2	1:C:181:SER:O	1.67	1.37
2:D:279:VAL:O	2:D:282:THR:HG22	1.19	1.34
2:B:193:CYS:SG	4:B:501:SGM:S1	2.32	1.28
2:D:193:CYS:SG	4:D:501:SGM:S1	2.33	1.27
3:A:301:1RO:O1	3:A:301:1RO:H13	1.33	1.27
1:C:124:LEU:HD22	1:C:181:SER:O	1.26	1.10
1:A:71:HIS:NE2	1:A:73:GLU:OE2	1.87	1.06
2:D:279:VAL:O	2:D:282:THR:CG2	2.03	1.06
1:C:124:LEU:HD21	1:C:181:SER:O	1.47	1.06
3:A:301:1RO:C2	3:A:301:1RO:O1	2.08	1.01
3:C:301:1RO:H13	3:C:301:1RO:O1	1.64	0.96
3:C:301:1RO:C2	3:C:301:1RO:O1	2.15	0.94
1:C:216:PHE:HB3	1:C:221:THR:HG22	1.47	0.94
3:A:301:1RO:C13	3:A:301:1RO:H13	2.05	0.86
3:A:301:1RO:N2	3:A:301:1RO:C19	2.37	0.83
1:C:224:GLU:OE2	1:C:231:THR:OG1	1.96	0.83
1:C:296:LEU:O	1:C:297:ARG:HG3	1.80	0.82
1:C:227:TRP:O	1:C:230:VAL:HG23	1.83	0.79
1:A:73:GLU:O	1:A:73:GLU:CG	2.30	0.78
1:A:13:GLY:HA3	3:A:301:1RO:H2	1.64	0.77
3:C:301:1RO:C19	3:C:301:1RO:N2	2.43	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:VAL:O	1:C:225:VAL:CG2	2.35	0.75
1:A:73:GLU:OE2	1:A:73:GLU:HA	1.86	0.74
1:C:14:THR:HG22	1:C:15:TYR:HD2	1.53	0.73
1:C:225:VAL:HG22	1:C:225:VAL:O	1.91	0.70
1:A:73:GLU:O	1:A:73:GLU:CD	2.29	0.70
1:A:60:HIS:HD2	1:A:62:ASN:H	1.41	0.68
3:C:301:1RO:C13	3:C:301:1RO:H13	2.23	0.67
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.24	0.67
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.77	0.66
1:A:73:GLU:C	1:A:73:GLU:CD	2.51	0.65
1:C:36:ARG:CG	1:C:36:ARG:HH21	2.09	0.65
1:C:14:THR:HG21	1:C:147:GLY:HA3	1.79	0.65
1:A:60:HIS:CD2	1:A:62:ASN:H	2.15	0.64
1:C:60:HIS:CD2	1:C:62:ASN:H	2.15	0.64
1:A:71:HIS:NE2	1:A:73:GLU:HA	2.14	0.63
1:C:36:ARG:HG3	1:C:36:ARG:HH21	1.64	0.62
1:A:73:GLU:O	1:A:73:GLU:HG3	1.98	0.62
1:C:227:TRP:HB3	1:C:230:VAL:HG21	1.81	0.61
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.82	0.61
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.83	0.60
1:A:294:PRO:HG2	1:A:296:LEU:HD22	1.83	0.60
1:C:223:ASP:OD1	1:C:226:VAL:HG12	2.02	0.59
1:C:82:PHE:CD2	1:C:83:LEU:O	2.55	0.59
1:A:73:GLU:CA	1:A:73:GLU:OE2	2.51	0.58
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.86	0.58
2:D:282:THR:O	2:D:283:ASP:HB2	2.03	0.58
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.86	0.57
1:C:221:THR:HG21	1:C:241:PRO:O	2.05	0.57
1:C:91:MET:HG2	1:C:99:ILE:HD11	1.87	0.56
1:A:82:PHE:CD2	1:A:83:LEU:O	2.59	0.56
3:A:301:1RO:C2	3:A:301:1RO:C13	2.76	0.56
1:C:296:LEU:O	1:C:297:ARG:CG	2.53	0.56
1:C:131[A]:GLN:O	3:C:301:1RO:H4	2.05	0.55
1:A:127:ASP:OD1	1:A:165:THR:HG23	2.07	0.55
2:D:193:CYS:SG	4:D:501:SGM:C1	2.94	0.55
1:A:71:HIS:CE1	1:A:73:GLU:OE2	2.57	0.54
1:A:53:SER:HB3	2:B:304:PHE:O	2.07	0.54
1:C:127:ASP:OD1	1:C:165:THR:HG23	2.08	0.53
1:C:82:PHE:CE2	1:C:83:LEU:O	2.62	0.53
1:C:131[B]:GLN:O	3:C:301:1RO:H4	2.07	0.53
1:C:36:ARG:NH2	1:C:36:ARG:HG3	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:OD1	1:C:223:ASP:C	2.48	0.51
1:A:131[A]:GLN:H	1:A:131[A]:GLN:CD	2.13	0.51
1:A:72:THR:O	1:A:74:ASN:N	2.45	0.50
1:A:198:THR:O	1:A:199:ARG:HB2	2.11	0.50
1:A:175:LEU:HB2	1:A:233:MET:HE1	1.93	0.50
1:A:73:GLU:O	1:A:73:GLU:OE1	2.30	0.50
1:C:223:ASP:O	1:C:223:ASP:OD1	2.30	0.50
1:C:45:PRO:HB2	1:C:47:THR:HG22	1.93	0.49
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.94	0.49
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.47	0.49
1:C:60:HIS:HD2	1:C:62:ASN:H	1.59	0.49
1:A:131[A]:GLN:O	3:A:301:1RO:H4	2.12	0.49
3:A:301:1RO:N2	3:A:301:1RO:C23	2.76	0.49
1:A:51:GLU:O	1:A:55:LEU:HB2	2.14	0.48
1:A:129:LYS:NZ	1:A:165:THR:HG21	2.29	0.47
1:C:216:PHE:O	1:C:219:LEU:O	2.32	0.47
3:C:301:1RO:N2	3:C:301:1RO:C23	2.78	0.46
1:A:74:ASN:HD22	1:A:74:ASN:HA	1.39	0.46
2:B:323:GLN:HA	2:B:324:PRO:HA	1.66	0.46
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.96	0.46
2:D:347:TYR:OH	2:D:394:LEU:HA	2.16	0.46
1:A:131[A]:GLN:OE1	1:A:131[A]:GLN:N	2.28	0.46
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.98	0.46
2:D:414:LYS:HG2	2:D:423:LEU:HG	1.98	0.46
1:A:97:THR:OG1	1:A:98:GLY:N	2.49	0.45
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.99	0.45
2:D:282:THR:O	2:D:285:THR:OG1	2.29	0.45
2:B:395:HIS:HE1	2:B:427:PRO:O	2.00	0.45
1:C:221:THR:CG2	1:C:243:TRP:H	2.29	0.45
1:A:137:THR:HG22	1:A:296:LEU:HD21	1.98	0.44
2:D:404:HIS:CE1	2:D:406:GLN:HG2	2.52	0.44
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.82	0.44
2:D:344:ALA:HB1	2:D:348:LEU:HD22	2.00	0.43
2:D:345:ASP:HA	2:D:346:PRO:HA	1.80	0.43
2:B:192:LYS:HB3	4:B:501:SGM:H31	2.00	0.43
1:A:51:GLU:HG3	1:A:55:LEU:HD22	2.00	0.42
2:B:345:ASP:HA	2:B:346:PRO:HA	1.75	0.42
1:C:129:LYS:HZ3	1:C:165:THR:HG21	1.84	0.42
1:C:14:THR:HG22	1:C:15:TYR:CD2	2.44	0.42
2:D:203:GLN:HA	2:D:204:PRO:HD3	1.84	0.41
1:A:14:THR:HG21	1:A:147:GLY:HA3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:ND1	2:D:300:LYS:HE2	2.36	0.41
1:A:127:ASP:OD1	1:A:165:THR:CG2	2.68	0.41
2:D:193:CYS:SG	4:D:501:SGM:H12	2.61	0.41
1:A:266:MET:O	1:A:274:ARG:HD3	2.21	0.41
2:B:281:ILE:HG13	2:B:281:ILE:H	1.74	0.41
1:C:51:GLU:O	1:C:55:LEU:HB2	2.21	0.41
2:B:347:TYR:OH	2:B:394:LEU:HA	2.21	0.40
2:D:280:TYR:C	2:D:282:THR:H	2.25	0.40
1:A:131[B]:GLN:O	3:A:301:IRO:H4	2.20	0.40
1:A:115:LEU:HD21	1:A:185:ASP:HB3	2.03	0.40
1:A:129:LYS:HD3	1:A:165:THR:CG2	2.51	0.40
1:A:81:GLU:O	3:A:301:IRO:H9	2.21	0.40
1:C:155:PRO:HD2	2:D:316:THR:HB	2.02	0.40
2:D:346:PRO:O	2:D:349:LYS:HG2	2.21	0.40
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.03	0.40
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.36	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	291/300 (97%)	276 (95%)	13 (4%)	2 (1%)	22	32
1	C	298/300 (99%)	286 (96%)	11 (4%)	1 (0%)	41	55
2	B	255/258 (99%)	249 (98%)	6 (2%)	0	100	100
2	D	254/258 (98%)	251 (99%)	2 (1%)	1 (0%)	34	48
All	All	1098/1116 (98%)	1062 (97%)	32 (3%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	C	164	VAL
1	A	164	VAL
2	D	283	ASP

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	261/263 (99%)	248 (95%)	13 (5%)	24	40
1	C	264/263 (100%)	247 (94%)	17 (6%)	17	28
2	B	231/232 (100%)	225 (97%)	6 (3%)	46	66
2	D	230/232 (99%)	219 (95%)	11 (5%)	25	41
All	All	986/990 (100%)	939 (95%)	47 (5%)	26	41

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	61	PRO
1	A	74	ASN
1	A	75	LYS
1	A	88	LYS
1	A	96	LEU
1	A	97	THR
1	A	122	ARG
1	A	150	ARG
1	A	165	THR
1	A	177	CYS
1	A	178	LYS
1	A	287	GLN
2	B	179	HIS
2	B	232	LEU
2	B	283	ASP
2	B	292	LEU
2	B	323	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	378	ARG
1	C	36	ARG
1	C	37	LEU
1	C	40	GLU
1	C	55	LEU
1	C	71	HIS
1	C	72	THR
1	C	83	LEU
1	C	101	LEU
1	C	103	LEU
1	C	122	ARG
1	C	131[A]	GLN
1	C	131[B]	GLN
1	C	150	ARG
1	C	202	LEU
1	C	225	VAL
1	C	249	SER
1	C	281	LEU
2	D	179	HIS
2	D	196	LYS
2	D	223	GLU
2	D	232	LEU
2	D	281	ILE
2	D	283	ASP
2	D	285	THR
2	D	292	LEU
2	D	384	LEU
2	D	386	SER
2	D	417	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	74	ASN
1	A	287	GLN
2	B	179	HIS
2	B	254	GLN
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	60	HIS
1	C	119	HIS
1	C	246	GLN
2	D	254	GLN
2	D	323	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	A	160	1	8,10,11	0.71	0	10,14,16	1.04	0
1	TPO	C	160	1	8,10,11	0.75	0	10,14,16	0.99	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	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1RO	A	301	-	27,27,27	3.11	3 (11%)	32,37,37	4.97	12 (37%)
4	SGM	D	501	-	5,5,5	0.36	0	5,5,5	0.49	0
4	SGM	B	501	-	5,5,5	0.33	0	5,5,5	0.61	0
3	1RO	C	301	-	27,27,27	3.06	4 (14%)	32,37,37	4.14	13 (40%)

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	1RO	A	301	-	-	3/7/21/21	0/4/4/4
4	SGM	D	501	-	-	0/4/4/4	-
4	SGM	B	501	-	-	1/4/4/4	-
3	1RO	C	301	-	-	3/7/21/21	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	1RO	C11-C12	13.95	1.50	1.34
3	C	301	1RO	C11-C12	13.78	1.49	1.34
3	C	301	1RO	C3-C4	4.25	1.48	1.42
3	A	301	1RO	C3-C4	4.05	1.48	1.42
3	A	301	1RO	C13-N2	-4.01	1.30	1.37
3	C	301	1RO	C13-N2	-2.70	1.33	1.37
3	C	301	1RO	O1-C13	2.48	1.27	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	1RO	N3-C15-N2	-14.98	112.05	124.05
3	C	301	1RO	N3-C15-N2	-11.66	114.72	124.05
3	A	301	1RO	C12-C13-N2	10.73	119.18	113.56
3	A	301	1RO	S1-C15-N3	9.91	131.82	121.33
3	A	301	1RO	C1-C11-C12	-9.73	117.64	130.94
3	C	301	1RO	C1-C11-C12	-9.62	117.78	130.94
3	C	301	1RO	C12-C13-N2	9.21	118.38	113.56
3	A	301	1RO	C22-C21-S2	-8.44	106.13	112.98
3	C	301	1RO	C22-C21-S2	-8.23	106.30	112.98
3	A	301	1RO	C13-C12-S1	-7.65	104.89	109.12
3	C	301	1RO	S1-C15-N3	7.44	129.21	121.33
3	A	301	1RO	O1-C13-C12	6.54	126.42	122.51
3	C	301	1RO	C13-C12-S1	-6.34	105.62	109.12
3	A	301	1RO	O1-C13-N2	-4.92	114.40	124.36
3	A	301	1RO	C11-C12-C13	4.74	127.05	122.31
3	C	301	1RO	C11-C12-C13	4.35	126.66	122.31
3	C	301	1RO	O1-C13-N2	-3.36	117.56	124.36
3	A	301	1RO	C18-N3-C15	-2.91	118.80	122.04
3	C	301	1RO	C9-N1-C4	2.82	121.30	116.93
3	C	301	1RO	C5-C4-N1	2.69	122.94	118.52
3	A	301	1RO	C9-N1-C4	2.67	121.06	116.93
3	A	301	1RO	C5-C4-N1	2.62	122.83	118.52
3	C	301	1RO	O1-C13-C12	2.59	124.06	122.51
3	C	301	1RO	C3-C4-N1	-2.40	118.47	122.02
3	C	301	1RO	C18-N3-C15	-2.08	119.73	122.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	1RO	C19-C18-N3-C15

Continued on next page...

Continued from previous page...

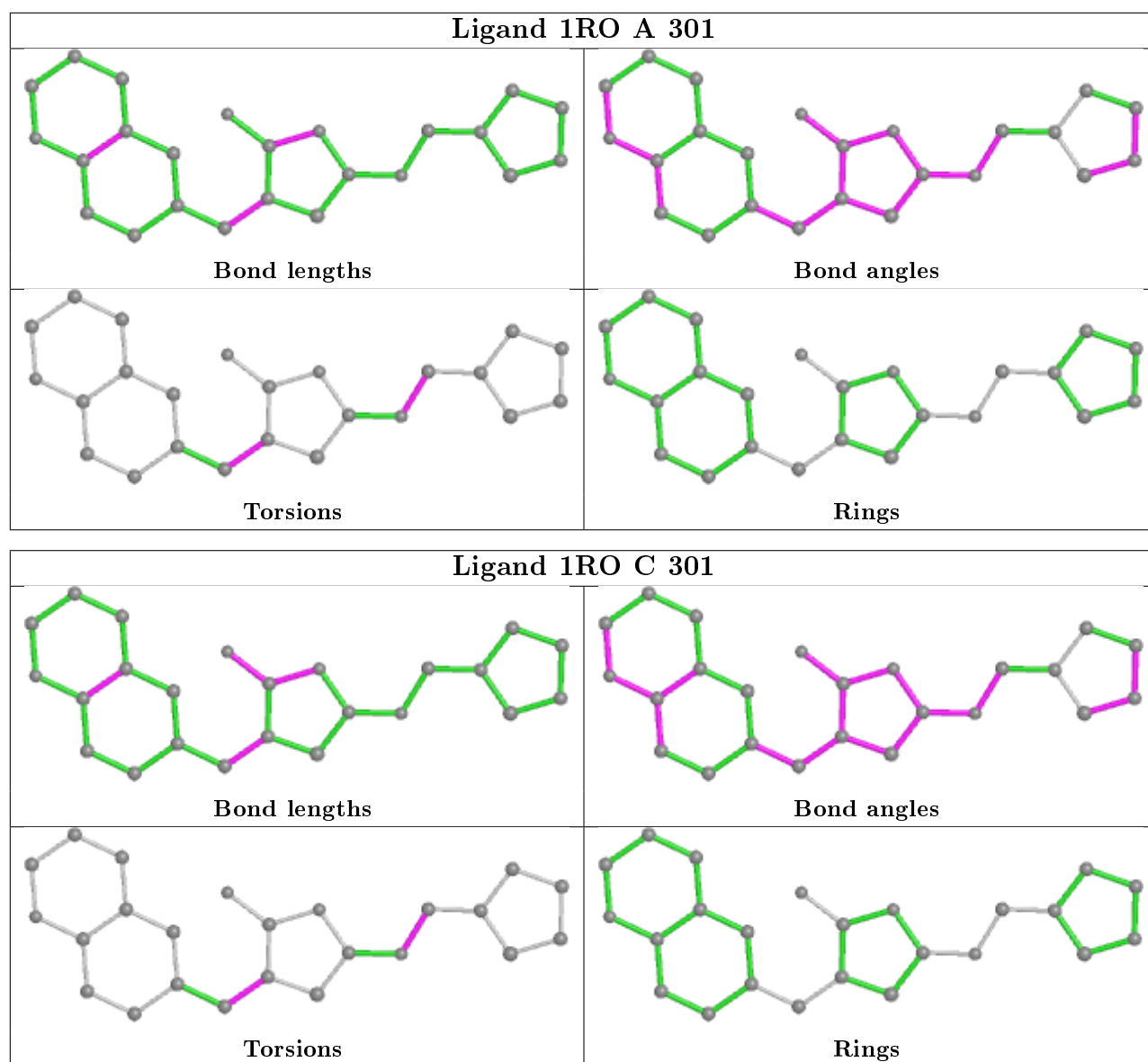
Mol	Chain	Res	Type	Atoms
3	A	301	1RO	C1-C11-C12-C13
3	C	301	1RO	C19-C18-N3-C15
3	C	301	1RO	C1-C11-C12-C13
3	A	301	1RO	C1-C11-C12-S1
3	C	301	1RO	C1-C11-C12-S1
4	B	501	SGM	S1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	1RO	10	0
4	D	501	SGM	3	0
4	B	501	SGM	2	0
3	C	301	1RO	7	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 [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	294/300 (98%)	-0.18	7 (2%) 59 57	27, 39, 67, 77	0
1	C	299/300 (99%)	0.20	20 (6%) 17 16	39, 57, 84, 95	0
2	B	257/258 (99%)	-0.02	8 (3%) 49 47	30, 50, 73, 91	0
2	D	256/258 (99%)	0.37	30 (11%) 4 4	38, 63, 107, 128	0
All	All	1106/1116 (99%)	0.09	65 (5%) 22 21	27, 51, 89, 128	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	GLU	8.4
1	C	73	GLU	5.8
1	C	39	THR	5.0
2	D	416	SER	4.9
1	A	73	GLU	4.8
1	C	287	GLN	4.5
2	D	430	LEU	4.1
2	D	385	GLU	4.1
1	C	296	LEU	3.6
2	D	324	PRO	3.6
1	A	162[A]	GLU	3.5
1	A	74	ASN	3.5
2	D	423	LEU	3.3
2	D	284	ASP	3.3
1	A	96	LEU	3.1
2	D	311	VAL	3.1
2	B	432	LEU	3.1
2	D	337	GLY	3.0
2	B	403	GLN	3.0
2	D	323	GLN	3.0
1	C	0	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	201	LYS	2.9
1	C	162	GLU	2.9
2	D	428	GLU	2.8
2	D	358	ALA	2.7
2	D	367	VAL	2.7
2	B	341	LEU	2.7
2	D	414	LYS	2.7
1	A	36	ARG	2.7
2	D	233	HIS	2.7
1	C	41	THR	2.6
1	C	-1	GLY	2.6
1	C	12	GLU	2.6
2	B	323	GLN	2.6
2	D	419	HIS	2.5
2	D	336	LEU	2.5
1	C	-2	LEU	2.5
2	D	339	LEU	2.5
2	D	429	THR	2.5
1	C	36	ARG	2.4
2	D	368	THR	2.4
1	C	189	LEU	2.4
2	D	415	ASN	2.3
2	D	176	PRO	2.3
2	D	424	LEU	2.3
2	D	201	LYS	2.3
1	C	297	ARG	2.3
2	B	236	VAL	2.3
2	D	325	ALA	2.3
2	B	235	ALA	2.2
2	D	431	ASN	2.2
2	D	333	ALA	2.2
2	D	356	ALA	2.2
1	A	72	THR	2.2
1	C	178	LYS	2.1
1	C	187	TRP	2.1
1	C	256	ASP	2.1
1	C	74	ASN	2.1
1	C	257	GLU	2.1
2	B	359	ALA	2.1
2	D	355	ILE	2.1
1	A	97	THR	2.0
2	D	357	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	225	VAL	2.0
2	D	388	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.97	0.11	46,52,55,55	0
1	TPO	A	160	11/12	0.98	0.10	35,37,38,38	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

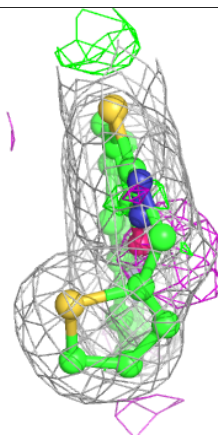
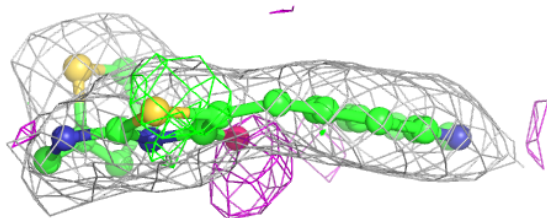
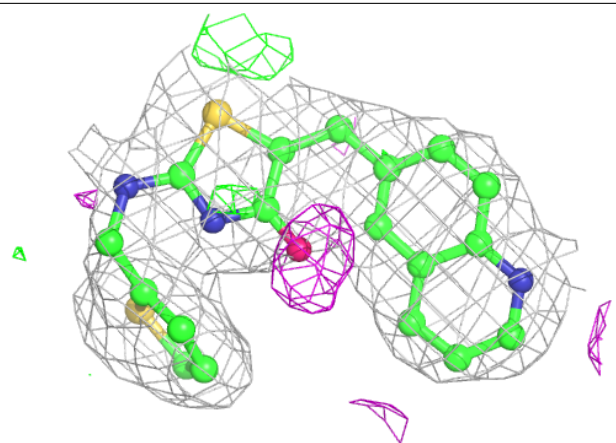
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SGM	D	501	6/6	0.91	0.24	58,60,61,61	0
3	1RO	A	301	24/24	0.92	0.15	38,45,50,50	0
4	SGM	B	501	6/6	0.93	0.19	49,51,51,52	0
3	1RO	C	301	24/24	0.93	0.13	49,56,57,58	0
5	MG	B	502	1/1	0.93	0.20	53,53,53,53	0

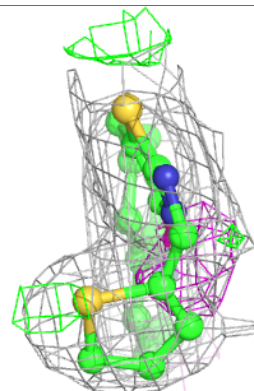
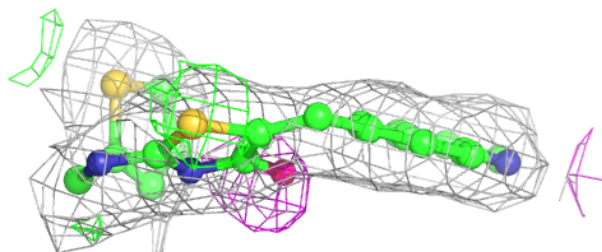
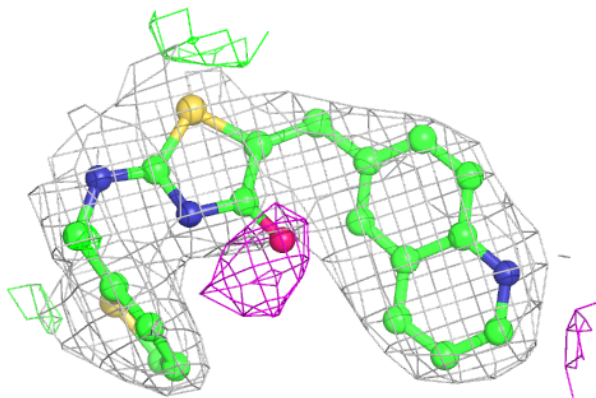
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1RO 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 1RO 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

There are no such residues in this entry.