Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 07:57 AM EDT

PDB ID	:	3DDP
Title	:	Structure of phosphorylated Thr160 CDK2/cyclin A in complex with the inhibitor CR8
Authors	:	Echalier, A.; Endicott, J.A.
Deposited on	:	2008-06-06
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

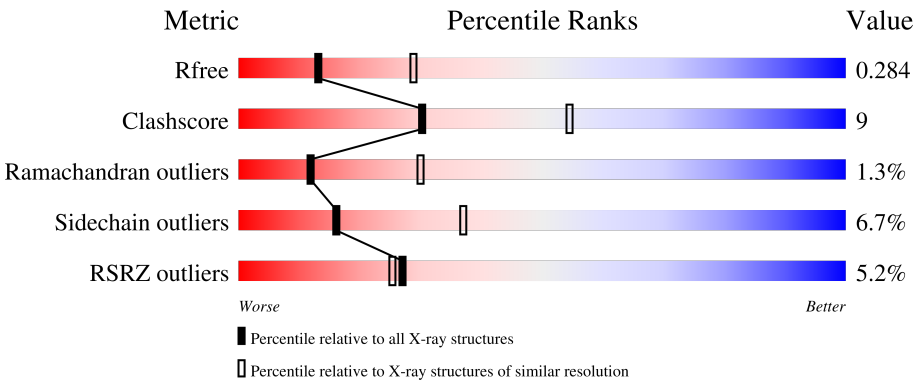
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	3%, 76%, 20%, •
1	C	299	10%, 70%, 25%, •
2	B	268	2%, 82%, 15%, • •
2	D	268	6%, 78%, 18%, •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9299 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
			Total	C	N	O	P	S			
1	A	298	2404	1559	409	427	1	8	0	1	0
1	C	299	2407	1562	409	427	1	8	0	0	0

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
			Total	C	N	O	S			
2	B	262	2118	1371	344	393	10	0	1	0
2	D	268	2172	1403	362	397	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	433	HIS	-	EXPRESSION TAG	UNP P30274
B	434	HIS	-	EXPRESSION TAG	UNP P30274
B	435	HIS	-	EXPRESSION TAG	UNP P30274
B	436	HIS	-	EXPRESSION TAG	UNP P30274
B	437	HIS	-	EXPRESSION TAG	UNP P30274
B	438	HIS	-	EXPRESSION TAG	UNP P30274
D	433	HIS	-	EXPRESSION TAG	UNP P30274
D	434	HIS	-	EXPRESSION TAG	UNP P30274
D	435	HIS	-	EXPRESSION TAG	UNP P30274
D	436	HIS	-	EXPRESSION TAG	UNP P30274

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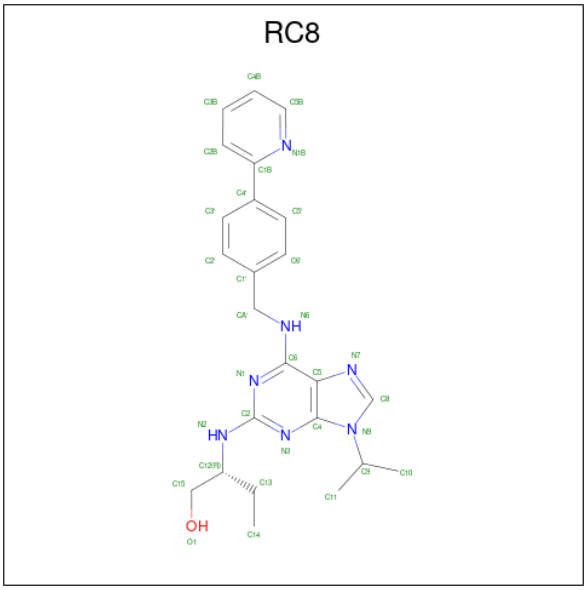
Chain	Residue	Modelled	Actual	Comment	Reference
D	437	HIS	-	EXPRESSION TAG	UNP P30274
D	438	HIS	-	EXPRESSION TAG	UNP P30274

- Molecule 3 is (2R)-2-({9-(1-methylethyl)-6-[(4-pyridin-2-ylbenzyl)amino]-9H-purin-2-yl}amino)butan-1-ol (three-letter code: RC8) (formula: $C_{24}H_{29}N_7O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	24	7	1		
3	C	1	Total	C	N	O	0	0
			32	24	7	1		

- Molecule 4 is water.

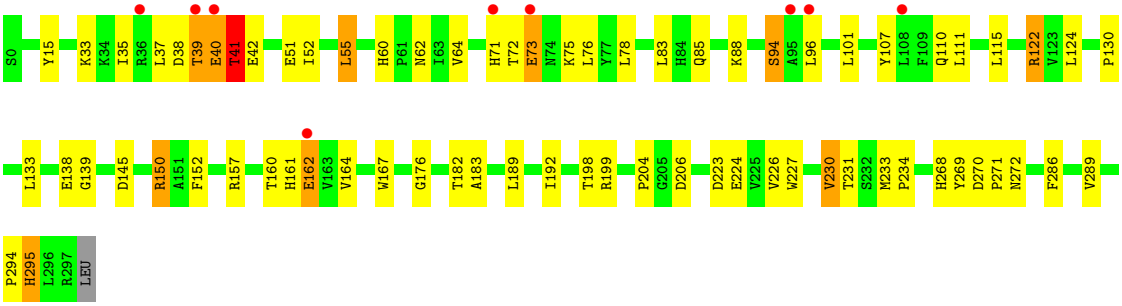
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	28	Total	O	0	0
			28	28		
4	C	33	Total	O	0	0
			33	33		
4	D	20	Total	O	0	0
			20	20		

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.

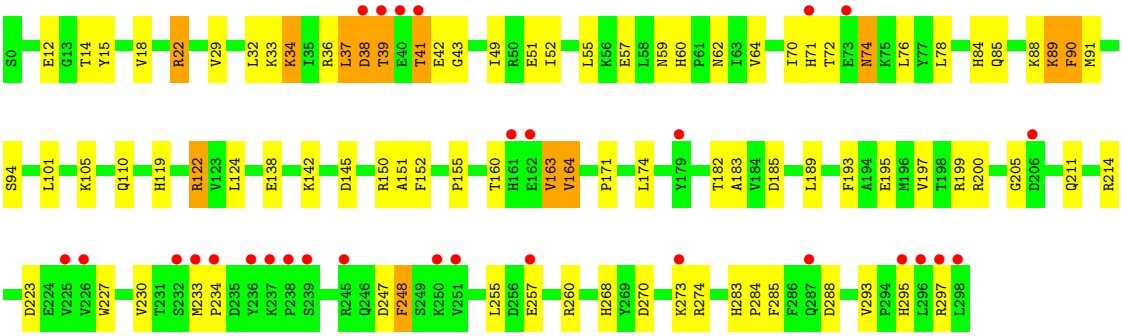
• Molecule 1: Cell division protein kinase 2

Chain A:



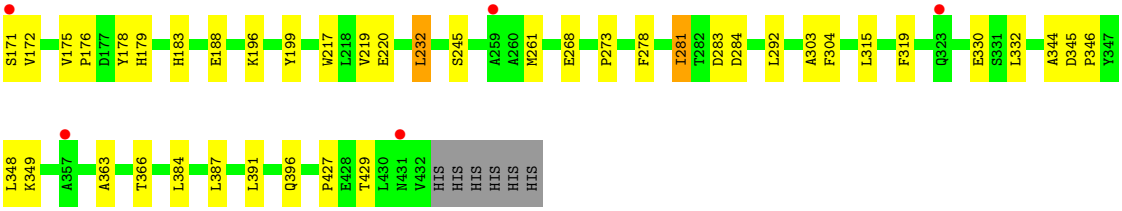
• Molecule 1: Cell division protein kinase 2

Chain C:



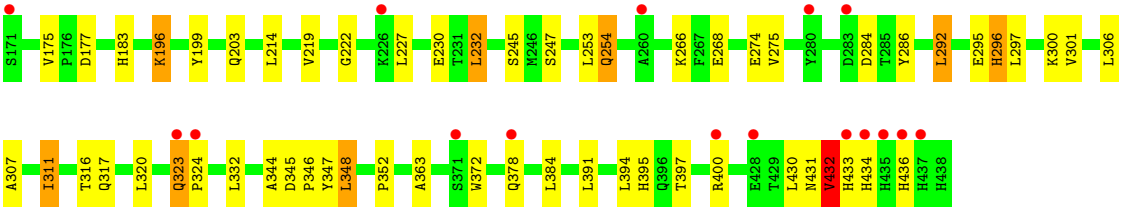
• Molecule 2: Cyclin-A2

Chain B:



• Molecule 2: Cyclin-A2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.32Å 135.16Å 168.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.70) 93.0 (19.98-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.270 0.236 , 0.284	Depositor DCC
R_{free} test set	2225 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9299	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: RC8, 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	0.50	0/2457	0.62	0/3333
1	C	0.44	0/2457	0.61	0/3333
2	B	0.44	0/2171	0.59	0/2952
2	D	0.40	0/2228	0.56	0/3030
All	All	0.45	0/9313	0.60	0/12648

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	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	70	ILE	Peptide
1	C	89	LYS	Peptide

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	2404	0	2449	53	0
1	C	2407	0	2454	67	0
2	B	2118	0	2136	24	0
2	D	2172	0	2172	39	0
3	A	32	0	29	2	0
3	C	32	0	29	2	0
4	A	53	0	0	3	0
4	B	28	0	0	3	0
4	C	33	0	0	6	0
4	D	20	0	0	3	0
All	All	9299	0	9269	171	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 (171) 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:41:THR:CB	1:C:42:GLU:HA	1.77	1.14
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.32	1.12
1:C:41:THR:HB	1:C:42:GLU:HA	1.39	1.04
1:A:41:THR:HA	4:A:336:HOH:O	1.62	0.99
1:C:41:THR:HB	1:C:42:GLU:CA	2.00	0.89
1:C:41:THR:HB	1:C:43:GLY:H	1.38	0.86
1:C:38:ASP:O	1:C:39:THR:HG22	1.79	0.83
1:A:37:LEU:HB3	1:A:39:THR:H	1.42	0.81
1:A:85:GLN:HA	3:A:299:RC8:HA'A	1.62	0.81
1:C:42:GLU:HB3	2:D:275:VAL:HG23	1.64	0.80
1:C:41:THR:HB	1:C:43:GLY:N	1.97	0.79
1:C:41:THR:OG1	1:C:42:GLU:HA	1.84	0.78
1:A:37:LEU:HA	1:A:38:ASP:CB	2.15	0.76
1:A:37:LEU:HA	1:A:38:ASP:HB3	1.66	0.75
1:C:85:GLN:HE21	1:C:90:PHE:HB2	1.53	0.74
1:C:39:THR:HG23	1:C:41:THR:HA	1.69	0.74
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.17	0.72
1:A:60:HIS:CD2	1:A:62:ASN:H	2.09	0.70
2:D:284:ASP:HB2	4:D:37:HOH:O	1.92	0.70
2:B:179:HIS:HB2	4:B:450:HOH:O	1.93	0.69
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.75	0.69
1:C:41:THR:CB	1:C:42:GLU:CA	2.58	0.67
1:A:39:THR:HG23	1:A:40:GLU:H	1.59	0.67
1:C:51:GLU:O	1:C:55:LEU:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:TRP:O	1:A:230:VAL:HG22	1.96	0.65
1:C:60:HIS:HE1	4:C:321:HOH:O	1.80	0.65
1:C:84:HIS:HB2	4:C:304:HOH:O	1.96	0.65
1:C:22:ARG:HG2	4:C:302:HOH:O	1.96	0.65
1:C:227:TRP:O	1:C:230:VAL:HG23	1.97	0.65
1:C:37:LEU:HA	1:C:38:ASP:C	2.19	0.63
2:B:183:HIS:HE1	4:B:448:HOH:O	1.80	0.63
1:A:15:TYR:CE2	1:A:35:ILE:HG12	2.34	0.62
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.80	0.62
2:D:175:VAL:O	2:D:175:VAL:HG13	1.98	0.62
1:C:155:PRO:HD3	2:D:320:LEU:HD21	1.81	0.62
1:C:60:HIS:CD2	1:C:62:ASN:H	2.17	0.62
1:C:119:HIS:CD2	1:C:182:THR:HB	2.35	0.61
1:C:71:HIS:HD2	1:C:76:LEU:HD13	1.67	0.58
2:D:347:TYR:HH	2:D:397:THR:HG1	1.51	0.58
1:A:39:THR:HG23	1:A:40:GLU:N	2.21	0.56
1:C:248:PHE:HB3	1:C:260:ARG:HD2	1.87	0.56
2:B:366:THR:HG23	2:B:427:PRO:HD3	1.87	0.56
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.87	0.56
1:C:42:GLU:HB3	2:D:275:VAL:CG2	2.34	0.55
1:C:14:THR:HG22	1:C:15:TYR:H	1.70	0.55
2:D:431:ASN:O	2:D:432:VAL:HG13	2.06	0.55
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.42	0.54
1:C:60:HIS:HD2	1:C:62:ASN:H	1.55	0.54
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.90	0.54
1:A:51:GLU:HG3	1:A:55:LEU:HD22	1.90	0.54
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.88	0.54
2:D:297:LEU:O	2:D:301:VAL:HG23	2.08	0.53
1:C:85:GLN:NE2	1:C:90:PHE:HB2	2.22	0.53
1:C:205:GLY:HA2	1:C:214:ARG:HE	1.72	0.53
1:A:176:GLY:O	1:A:234:PRO:HG2	2.09	0.53
2:D:214:LEU:HD22	2:D:253:LEU:HG	1.90	0.53
1:C:59:ASN:HB2	4:C:305:HOH:O	2.08	0.52
1:C:122:ARG:HD2	1:C:122:ARG:O	2.09	0.52
1:A:15:TYR:HE2	1:A:35:ILE:HG12	1.74	0.52
1:A:37:LEU:CB	1:A:39:THR:H	2.17	0.52
1:A:64:VAL:HG21	3:A:299:RC8:H10A	1.90	0.52
2:D:372:TRP:HB3	2:D:384:LEU:HD13	1.92	0.52
1:A:94:SER:O	1:A:199:ARG:HD3	2.10	0.51
1:C:39:THR:HG23	1:C:41:THR:CA	2.38	0.51
2:D:311:ILE:HG22	2:D:352:PRO:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.25	0.51
1:A:161:HIS:CD2	4:A:346:HOH:O	2.64	0.50
1:C:64:VAL:HG21	3:C:299:RC8:H10A	1.92	0.50
1:C:34:LYS:NZ	1:C:36:ARG:HH21	2.08	0.50
1:A:272:ASN:CG	2:B:171:SER:OG	2.51	0.49
2:B:303:ALA:O	2:B:304:PHE:HB2	2.11	0.49
2:B:387:LEU:O	2:B:391:LEU:HB2	2.13	0.49
2:D:431:ASN:O	2:D:432:VAL:HG22	2.13	0.49
1:A:122:ARG:O	1:A:122:ARG:HD2	2.13	0.49
1:C:57:GLU:OE2	2:D:307:ALA:HB3	2.13	0.49
1:C:85:GLN:HA	3:C:299:RC8:HA'A	1.95	0.49
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.79	0.48
1:A:39:THR:O	1:A:41:THR:N	2.47	0.48
1:A:107:TYR:O	1:A:111:LEU:HG	2.13	0.48
2:B:171:SER:HG	2:B:172:VAL:H	1.60	0.48
1:C:41:THR:HB	1:C:42:GLU:C	2.35	0.48
1:A:39:THR:CG2	1:A:40:GLU:H	2.27	0.47
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.97	0.47
1:A:286:PHE:O	1:A:289:VAL:HG12	2.13	0.47
2:B:346:PRO:O	2:B:349:LYS:HG2	2.15	0.47
1:A:37:LEU:HB3	1:A:39:THR:N	2.22	0.47
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.97	0.47
2:B:175:VAL:HG13	2:B:175:VAL:O	2.15	0.47
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.30	0.47
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.98	0.46
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.78	0.46
1:A:157:ARG:HH22	2:B:268:GLU:HG3	1.79	0.46
1:C:193:PHE:O	1:C:197:VAL:HG23	2.16	0.46
2:D:296:HIS:CE1	4:D:72:HOH:O	2.69	0.46
2:D:196:LYS:HE2	2:D:199:TYR:HA	1.96	0.46
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.97	0.46
1:A:15:TYR:HE2	1:A:35:ILE:CD1	2.29	0.46
1:C:155:PRO:CD	2:D:316:THR:HG22	2.22	0.46
1:A:161:HIS:HD2	4:A:346:HOH:O	1.99	0.46
2:B:273:PRO:HG2	2:B:278:PHE:CE2	2.51	0.46
1:C:255:LEU:HD23	1:C:260:ARG:HG2	1.98	0.45
1:A:162:GLU:O	1:A:162:GLU:HG2	2.16	0.45
2:D:254:GLN:HB3	2:D:286:TYR:HE2	1.82	0.45
1:C:205:GLY:HA3	1:C:211:GLN:OE1	2.16	0.45
1:A:115:LEU:HD22	1:A:189:LEU:HD12	1.98	0.45
2:D:203:GLN:NE2	2:D:247:SER:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.52	0.45
1:A:150:ARG:HH21	1:A:160:TPO:P	2.40	0.45
2:B:217:TRP:O	2:B:220:GLU:HB2	2.16	0.45
1:C:88:LYS:HA	1:C:91:MET:HE2	1.99	0.45
1:C:119:HIS:HD2	4:C:332:HOH:O	2.00	0.44
1:C:270:ASP:HB3	1:C:273:LYS:HB2	1.99	0.44
2:B:183:HIS:CE1	4:B:448:HOH:O	2.62	0.44
2:D:254:GLN:HB3	2:D:286:TYR:CE2	2.53	0.44
1:C:60:HIS:CE1	4:C:321:HOH:O	2.62	0.44
2:D:266:LYS:NZ	2:D:295:GLU:OE2	2.36	0.44
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.53	0.43
2:B:175:VAL:HG22	2:B:178:TYR:HB2	2.00	0.43
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.99	0.43
2:D:222:GLY:HA2	2:D:227:LEU:HD12	2.00	0.43
1:C:122:ARG:O	1:C:151:ALA:HA	2.19	0.43
2:D:230:GLU:HA	2:D:230:GLU:OE1	2.19	0.43
1:C:183:ALA:HB1	1:C:274:ARG:HD2	2.00	0.43
2:D:345:ASP:HA	2:D:346:PRO:HA	1.77	0.43
1:C:38:ASP:OD1	1:C:39:THR:N	2.50	0.43
1:C:39:THR:HG23	1:C:41:THR:C	2.39	0.43
1:C:105:LYS:HG3	1:C:285:PHE:CE2	2.53	0.43
1:A:133:LEU:HD11	1:A:192:ILE:HD13	2.00	0.43
1:C:88:LYS:HA	1:C:91:MET:CE	2.48	0.43
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.02	0.43
2:D:323:GLN:HA	2:D:324:PRO:HA	1.81	0.43
1:C:62:ASN:HA	1:C:142:LYS:HG2	2.00	0.42
2:D:395:HIS:HB2	2:D:430:LEU:HD11	2.00	0.42
1:A:124:LEU:CD2	1:A:182:THR:HA	2.49	0.42
1:C:94:SER:O	1:C:199:ARG:HD2	2.19	0.42
1:A:15:TYR:CD2	1:A:35:ILE:HG12	2.55	0.42
2:D:400:ARG:HB3	4:D:31:HOH:O	2.20	0.42
2:D:292:LEU:HD12	2:D:292:LEU:HA	1.84	0.42
2:B:176:PRO:HA	2:B:179:HIS:HD2	1.85	0.41
1:A:94:SER:O	1:A:199:ARG:CD	2.69	0.41
1:C:49:ILE:HG23	2:D:306:LEU:HD12	2.01	0.41
2:D:394:LEU:HD12	2:D:394:LEU:HA	1.90	0.41
1:C:39:THR:CG2	1:C:41:THR:HA	2.44	0.41
1:A:33:LYS:HB3	1:A:78:LEU:HB2	2.03	0.41
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.55	0.41
1:A:230:VAL:HA	1:A:233:MET:SD	2.60	0.41
1:A:268:HIS:HD2	1:A:270:ASP:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:TYR:O	1:A:271:PRO:HD3	2.20	0.41
1:C:91:MET:SD	1:C:195:GLU:HG2	2.60	0.41
2:D:323:GLN:HA	2:D:323:GLN:HE21	1.85	0.41
1:A:295:HIS:ND1	1:A:295:HIS:N	2.68	0.41
1:C:283:HIS:HA	1:C:284:PRO:HD3	1.90	0.41
1:A:223:ASP:H	1:A:226:VAL:HG12	1.86	0.41
2:B:344:ALA:O	2:B:348:LEU:HB2	2.21	0.41
2:D:230:GLU:HG3	2:D:268:GLU:HG2	2.03	0.41
1:A:72:THR:HG22	1:A:73:GLU:H	1.86	0.41
2:B:281:ILE:H	2:B:281:ILE:HG13	1.62	0.41
2:B:315:LEU:HD23	2:B:315:LEU:HA	1.91	0.41
1:C:18:VAL:HA	1:C:32:LEU:O	2.21	0.41
1:C:171:PRO:HA	1:C:174:LEU:HD12	2.03	0.41
2:B:319:PHE:CZ	2:B:330:GLU:HA	2.56	0.41
2:D:433:HIS:CD2	2:D:433:HIS:H	2.38	0.41
1:C:33:LYS:HB2	1:C:78:LEU:HB2	2.03	0.40
1:A:183:ALA:HB2	2:B:172:VAL:HG21	2.04	0.40
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.29	0.40
1:A:139:GLY:HA2	1:A:294:PRO:HD3	2.02	0.40
1:C:42:GLU:OE2	2:D:274:GLU:HB2	2.21	0.40
1:A:41:THR:HB	1:A:42:GLU:H	1.63	0.40
1:A:198:THR:O	1:A:199:ARG:HB2	2.21	0.40
2:B:345:ASP:HA	2:B:346:PRO:HA	1.91	0.40
1:C:37:LEU:HG	1:C:74:ASN:O	2.22	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	296/299 (99%)	281 (95%)	9 (3%)	6 (2%)	7 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	296/299 (99%)	268 (90%)	21 (7%)	7 (2%)	6	15
2	B	261/268 (97%)	254 (97%)	6 (2%)	1 (0%)	34	60
2	D	266/268 (99%)	260 (98%)	5 (2%)	1 (0%)	34	60
All	All	1119/1134 (99%)	1063 (95%)	41 (4%)	15 (1%)	12	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	C	39	THR
1	C	295	HIS
2	D	432	VAL
1	A	39	THR
1	A	40	GLU
1	A	162	GLU
1	C	145	ASP
1	C	164	VAL
1	A	164	VAL
2	B	429	THR
1	C	38	ASP
1	A	145	ASP
1	C	297	ARG
1	C	234	PRO

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%)	249 (95%)	14 (5%)	22	48
1	C	263/263 (100%)	238 (90%)	25 (10%)	8	20
2	B	236/241 (98%)	224 (95%)	12 (5%)	24	50
2	D	241/241 (100%)	225 (93%)	16 (7%)	16	38
All	All	1003/1008 (100%)	936 (93%)	67 (7%)	16	37

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	55	LEU
1	A	73	GLU
1	A	75	LYS
1	A	83	LEU
1	A	94	SER
1	A	96	LEU
1	A	101	LEU
1	A	122	ARG
1	A	138	GLU
1	A	150	ARG
1	A	206	ASP
1	A	230	VAL
1	A	295	HIS
2	B	188	GLU
2	B	196	LYS
2	B	199	TYR
2	B	232	LEU
2	B	245	SER
2	B	261	MET
2	B	281	ILE
2	B	283	ASP
2	B	284	ASP
2	B	292	LEU
2	B	384	LEU
2	B	396	GLN
1	C	12	GLU
1	C	22	ARG
1	C	29	VAL
1	C	34	LYS
1	C	37	LEU
1	C	41	THR
1	C	72	THR
1	C	74	ASN
1	C	89	LYS
1	C	90	PHE
1	C	101	LEU
1	C	122	ARG
1	C	138	GLU
1	C	150	ARG
1	C	163	VAL
1	C	189	LEU

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Mol	Chain	Res	Type
1	C	200	ARG
1	C	223	ASP
1	C	233	MET
1	C	247	ASP
1	C	248	PHE
1	C	257	GLU
1	C	268	HIS
1	C	288	ASP
1	C	293	VAL
2	D	177	ASP
2	D	196	LYS
2	D	232	LEU
2	D	245	SER
2	D	254	GLN
2	D	292	LEU
2	D	296	HIS
2	D	300	LYS
2	D	311	ILE
2	D	323	GLN
2	D	348	LEU
2	D	378	GLN
2	D	391	LEU
2	D	432	VAL
2	D	434	HIS
2	D	436	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	265	GLN
1	A	268	HIS
2	B	179	HIS
2	B	254	GLN
2	B	317	GLN
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
1	C	60	HIS
1	C	62	ASN
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	85	GLN
1	C	110	GLN
1	C	119	HIS
1	C	265	GLN
2	D	317	GLN
2	D	323	GLN
2	D	378	GLN
2	D	434	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)

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	0.73	0	10,14,16	1.10	0
1	TPO	C	160	1	8,10,11	0.80	0	10,14,16	1.19	1 (10%)

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	-	1/9/11/13	-
1	TPO	C	160	1	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	TPO	OG1-P-O1P	-2.19	101.53	109.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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 monosaccharides 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	RC8	C	299	-	31,35,35	1.09	2 (6%)	33,48,48	2.35	11 (33%)
3	RC8	A	299	-	31,35,35	1.07	3 (9%)	33,48,48	2.44	12 (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
3	RC8	C	299	-	-	4/17/21/21	0/4/4/4
3	RC8	A	299	-	-	4/17/21/21	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	299	RC8	C6-C5	3.31	1.49	1.44
3	C	299	RC8	C6-N1	2.51	1.36	1.33
3	A	299	RC8	C11-C9	2.46	1.58	1.50
3	A	299	RC8	C6-C5	2.40	1.48	1.44
3	A	299	RC8	C10-C9	2.26	1.58	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	299	RC8	C9-N9-C4	-6.35	119.61	127.15
3	C	299	RC8	C8-N9-C9	6.34	131.65	125.42
3	A	299	RC8	C9-N9-C4	-5.99	120.04	127.15
3	C	299	RC8	C2-N3-C4	5.26	121.07	115.38
3	A	299	RC8	C8-N9-C9	5.23	130.55	125.42
3	A	299	RC8	C2-N3-C4	5.15	120.96	115.38
3	A	299	RC8	CA'-N6-C6	-3.71	118.17	123.05
3	A	299	RC8	C11-C9-N9	3.69	116.30	110.29
3	C	299	RC8	C4-C5-N7	-3.65	105.48	109.34
3	A	299	RC8	C2-N2-C12	-3.59	118.73	124.32
3	A	299	RC8	C4-C5-N7	-3.56	105.58	109.34
3	C	299	RC8	C5B-N1B-C1B	3.18	121.75	116.93
3	A	299	RC8	C5B-N1B-C1B	3.01	121.49	116.93
3	C	299	RC8	C2-N2-C12	-2.88	119.85	124.32
3	C	299	RC8	C2-N1-C6	2.64	122.85	116.36
3	A	299	RC8	C4B-C5B-N1B	-2.64	120.09	123.97
3	A	299	RC8	C10-C9-N9	2.62	114.55	110.29
3	C	299	RC8	C4B-C5B-N1B	-2.59	120.16	123.97
3	C	299	RC8	N3-C2-N1	-2.51	122.14	126.25
3	C	299	RC8	N2-C2-N1	2.31	120.71	117.09
3	A	299	RC8	N3-C2-N1	-2.31	122.48	126.25
3	A	299	RC8	C2-N1-C6	2.28	121.97	116.36
3	C	299	RC8	C1'-CA'-N6	-2.02	107.99	113.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	299	RC8	C13-C12-C15-O1
3	A	299	RC8	N2-C12-C15-O1
3	A	299	RC8	C15-C12-C13-C14
3	A	299	RC8	N2-C12-C13-C14
3	C	299	RC8	C13-C12-C15-O1
3	C	299	RC8	N2-C12-C15-O1
3	C	299	RC8	C15-C12-C13-C14
3	C	299	RC8	N2-C12-C13-C14

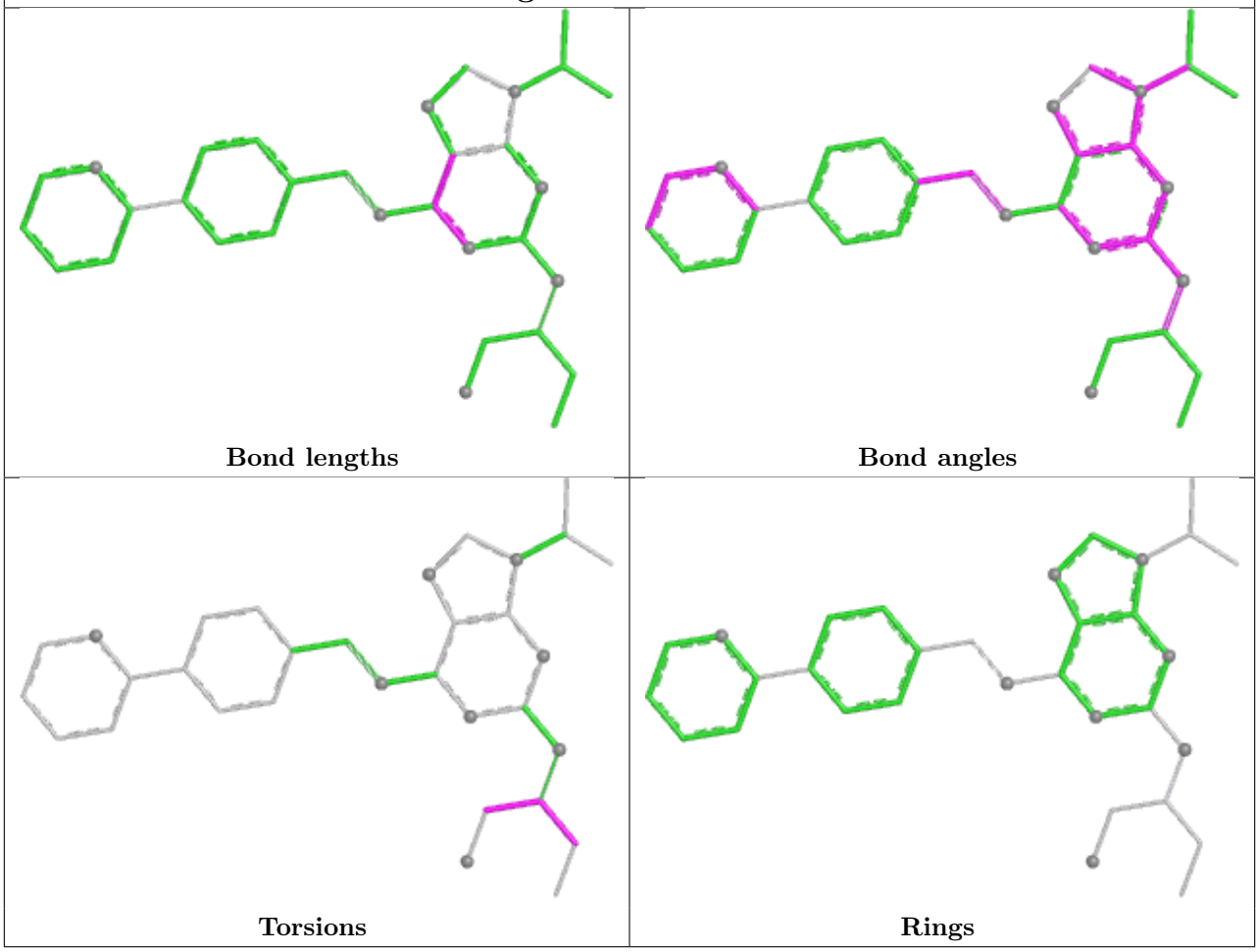
There are no ring outliers.

2 monomers are involved in 4 short contacts:

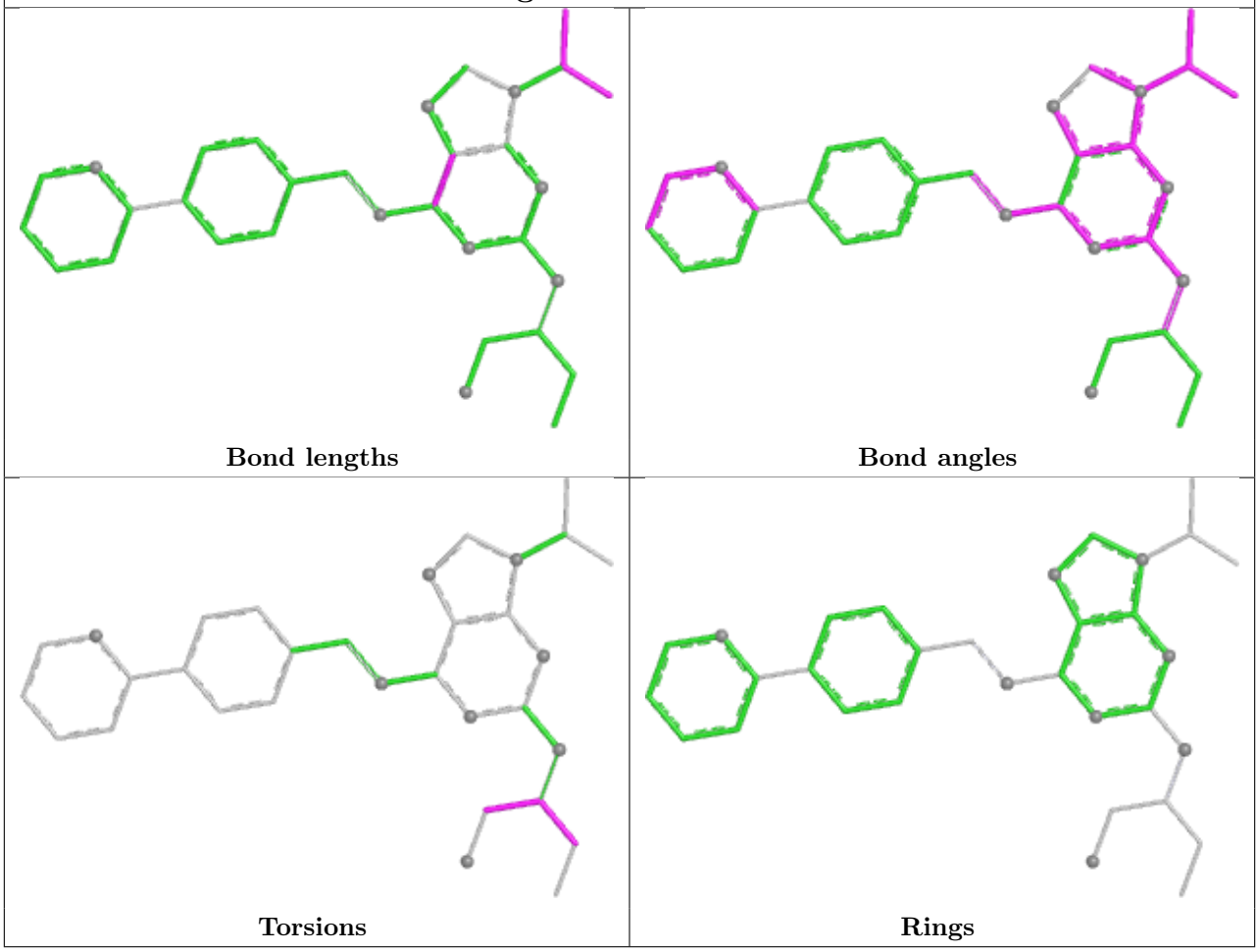
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	299	RC8	2	0
3	A	299	RC8	2	0

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 then 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.

Ligand RC8 C 299



Ligand RC8 A 299



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	297/299 (99%)	0.20	9 (3%) 50 51	42, 54, 67, 80	0
1	C	298/299 (99%)	0.28	29 (9%) 7 6	45, 55, 81, 115	0
2	B	262/268 (97%)	0.02	5 (1%) 66 69	41, 55, 66, 85	0
2	D	268/268 (100%)	0.17	16 (5%) 21 20	44, 57, 68, 82	0
All	All	1125/1134 (99%)	0.17	59 (5%) 27 25	41, 55, 73, 115	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	435	HIS	5.3
1	C	40	GLU	5.2
1	C	251	VAL	5.1
2	D	434	HIS	4.8
2	D	171	SER	4.4
1	C	297	ARG	4.4
1	C	225	VAL	4.1
1	C	238	PRO	4.0
1	C	295	HIS	4.0
2	B	171	SER	3.7
1	C	250	LYS	3.6
2	D	324	PRO	3.5
1	C	73	GLU	3.5
1	C	233	MET	3.5
2	D	433	HIS	3.4
2	D	280	TYR	3.3
1	C	226	VAL	3.3
1	C	71	HIS	3.2
1	C	239	SER	3.1
1	C	296	LEU	3.0
1	A	40	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	259	ALA	3.0
1	A	73	GLU	2.9
1	A	162	GLU	2.9
1	C	39	THR	2.9
1	C	245	ARG	2.9
2	D	428	GLU	2.8
1	C	298	LEU	2.8
2	D	226	LYS	2.8
1	C	232	SER	2.7
1	C	237	LYS	2.7
1	A	71	HIS	2.6
2	D	323	GLN	2.6
1	C	162	GLU	2.6
1	A	108	LEU	2.6
2	D	378	GLN	2.6
2	D	283	ASP	2.5
1	C	257	GLU	2.5
2	D	436	HIS	2.5
1	C	234	PRO	2.5
1	C	41	THR	2.5
1	C	287	GLN	2.4
1	A	36	ARG	2.4
2	B	323	GLN	2.4
1	C	179	TYR	2.3
1	A	95	ALA	2.3
1	C	38	ASP	2.3
1	C	206	ASP	2.3
2	D	371	SER	2.2
1	C	273	LYS	2.2
2	B	431	ASN	2.2
1	A	39	THR	2.2
2	B	357	ALA	2.2
2	D	260	ALA	2.2
1	C	161	HIS	2.1
1	A	96	LEU	2.1
1	C	236	TYR	2.1
2	D	400	ARG	2.0
2	D	437	HIS	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	0.96	0.14	47,51,53,53	0
1	TPO	A	160	11/12	0.99	0.14	49,53,57,57	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

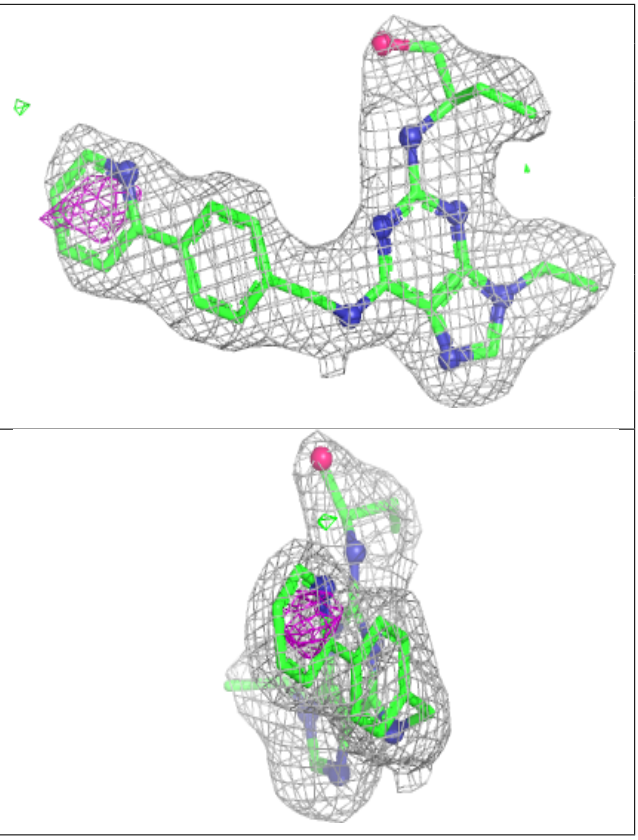
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RC8	C	299	32/32	0.85	0.23	51,56,62,62	0
3	RC8	A	299	32/32	0.86	0.22	43,47,55,55	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.

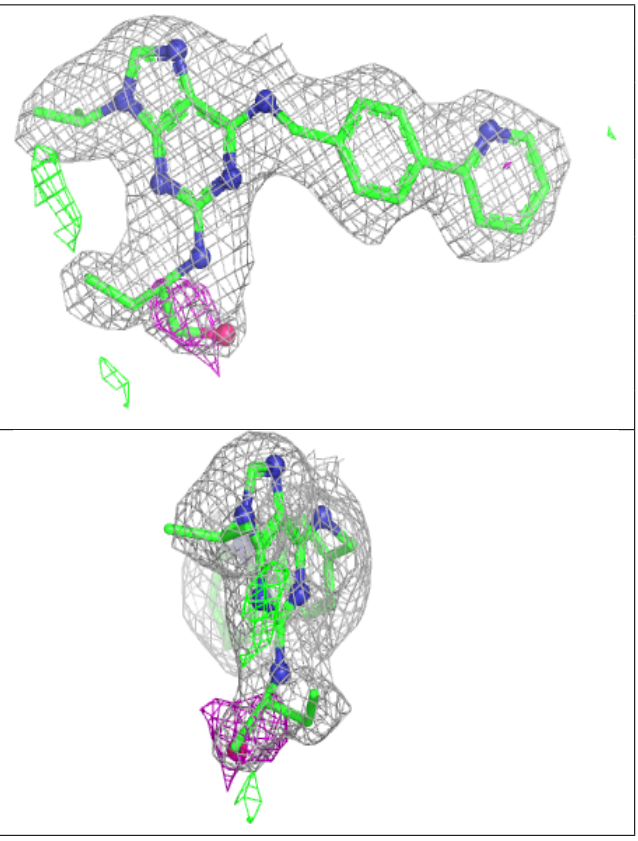
Electron density around RC8 C 299:

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



Electron density around RC8 A 299:

$2mF_o$-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.