



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 03:05 pm GMT

PDB ID : 1OGU  
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2/CYCLIN A COM-  
PLEXED WITH A 2-ARYLAMINO-4-CYCLOHEXYLMETHYL-5-NITROS  
O-6-AMINOPYRIMIDINE INHIBITOR  
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Deposited on : 2003-05-13  
Resolution : 2.60 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

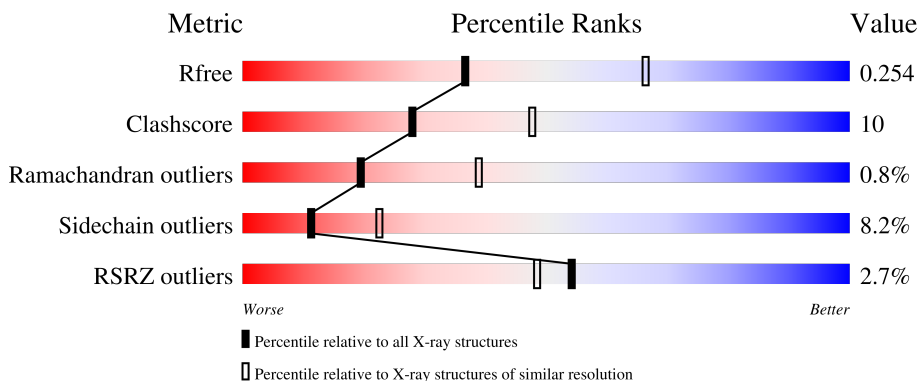
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	302	 2% 69% 26% . .
1	C	302	 3% 60% 27% . 10%
2	B	260	 2% 79% 17% . .
2	D	260	 3% 74% 21% . .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8893 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.

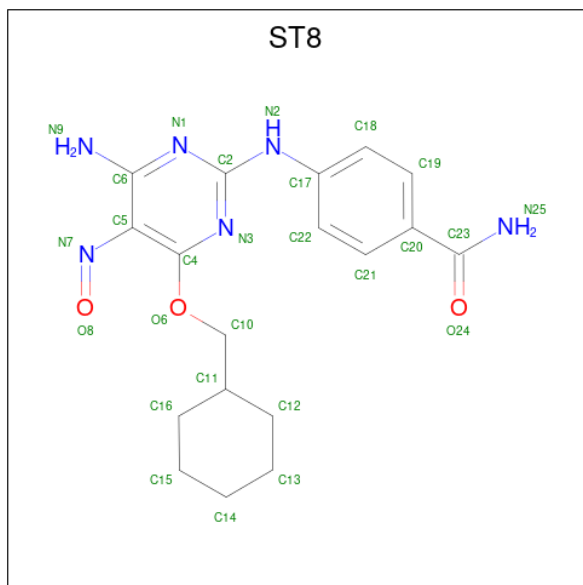
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	297	Total 2392	C 1554	N 409	O 420	P 1	S 8	0	1	0
1	C	273	Total 2185	C 1417	N 372	O 388	P 1	S 7	0	0	0

- Molecule 2 is a protein called CYCLIN A2.

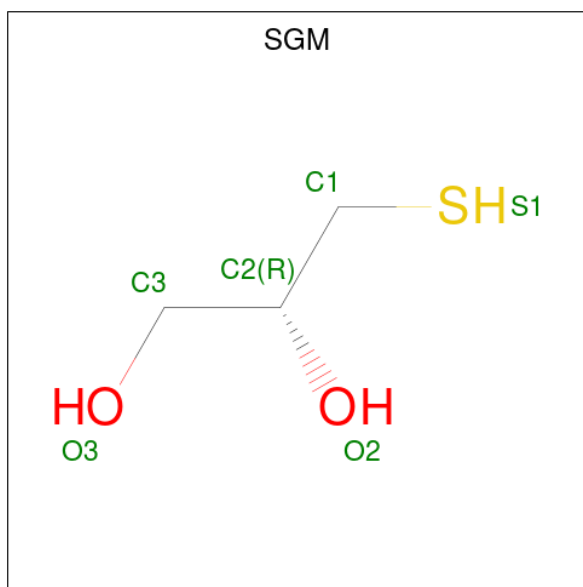
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	253	Total 2050	C 1331	N 335	O 373	S 11	0	1	0
2	D	255	Total 2066	C 1339	N 337	O 379	S 11	0	1	0

- Molecule 3 is 4-[[4-AMINO-6-(CYCLOHEXYLMETHOXY)-5-NITROSOPYRIMIDIN-2-YL]AMINO}BENZAMIDE (three-letter code: ST8) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	18	6	3		
3	C	1	Total	C	N	O	0	0
			27	18	6	3		

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>S).



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		

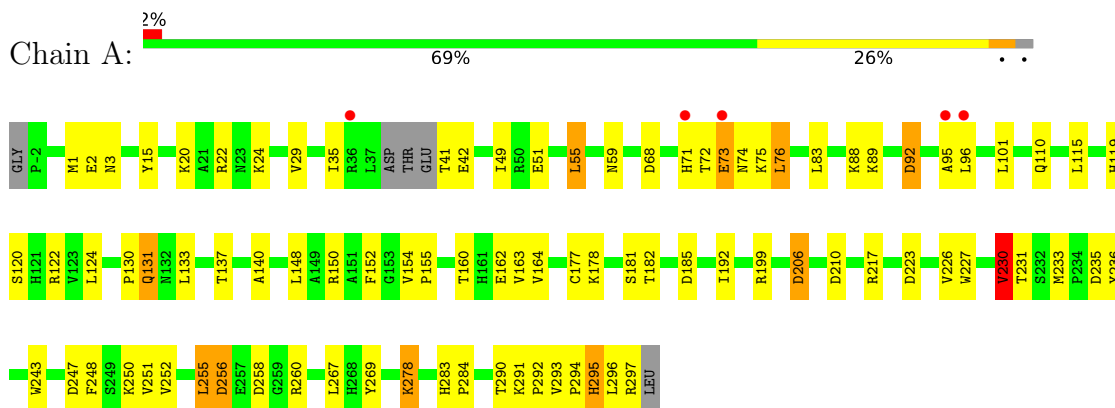
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total	O	0	0
			44	44		
5	B	37	Total	O	0	0
			37	37		
5	C	25	Total	O	0	0
			25	25		
5	D	28	Total	O	0	0
			28	28		

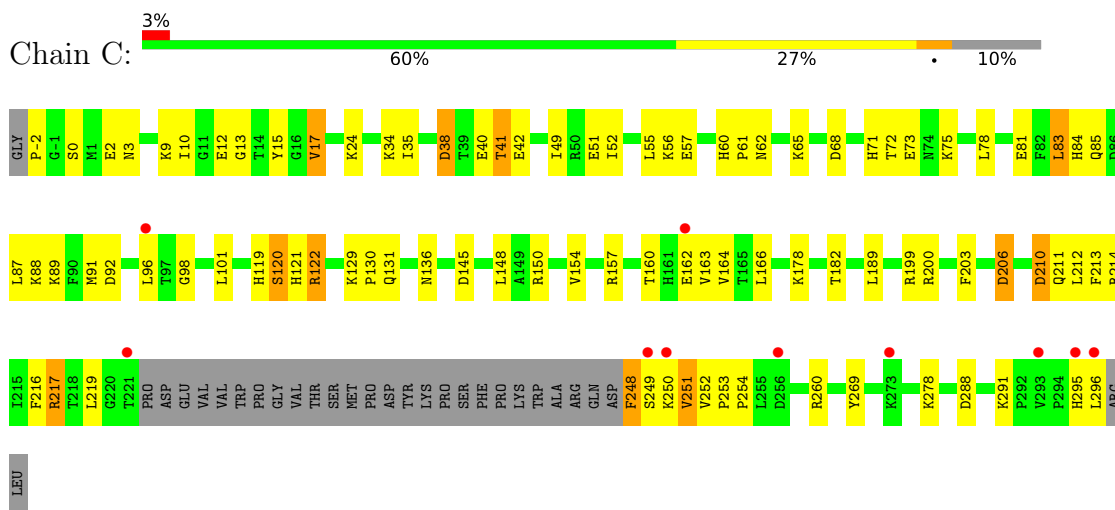
### 3 Residue-property plots [i](#)

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.

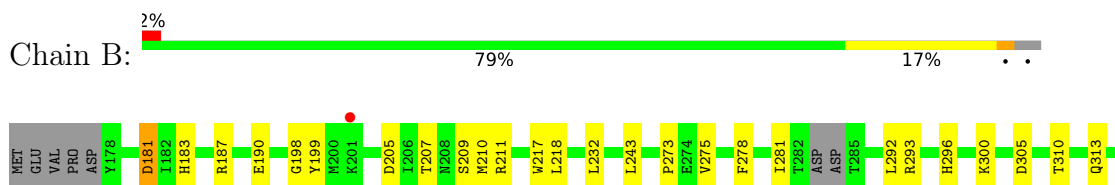
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

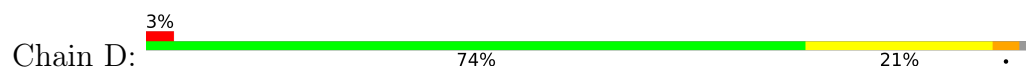


#### • Molecule 2: CYCLIN A2





● Molecule 2: CYCLIN A2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.84Å 133.68Å 148.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.60 32.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (100.00-2.60) 90.1 (32.60-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.198 , 0.260 0.194 , 0.254	Depositor DCC
$R_{free}$ test set	2076 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SGM, TPO, ST8

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	0.90	1/2447 (0.0%)	1.00	12/3317 (0.4%)
1	C	0.78	0/2224	0.91	6/3010 (0.2%)
2	B	0.83	0/2102	0.95	4/2851 (0.1%)
2	D	0.75	0/2119	0.90	5/2876 (0.2%)
All	All	0.82	1/8892 (0.0%)	0.94	27/12054 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	ASP	CB-CG	5.46	1.63	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	ASP	CB-CG-OD2	9.05	126.45	118.30
1	C	206	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	247	ASP	CB-CG-OD2	7.33	124.89	118.30
2	D	393	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	68	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	235	ASP	CB-CG-OD2	6.78	124.41	118.30
1	A	256	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	230	VAL	CB-CA-C	-6.53	99.00	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	ASP	CB-CG-OD2	6.34	124.01	118.30
2	B	343	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	92	ASP	CB-CG-OD2	6.27	123.94	118.30
1	C	92	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	210	ASP	CB-CG-OD2	6.04	123.74	118.30
2	D	205	ASP	CB-CG-OD2	5.89	123.61	118.30
1	C	288	ASP	CB-CG-OD2	5.78	123.50	118.30
2	D	247	SER	CB-CA-C	5.55	120.65	110.10
1	A	131	GLN	CA-CB-CG	5.45	125.40	113.40
2	B	187	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	D	181	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	258	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	432	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	206	ASP	CB-CG-OD2	5.25	123.03	118.30
2	B	205	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	96	LEU	CA-CB-CG	5.23	127.34	115.30
2	B	181	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	76	LEU	CA-CB-CG	5.06	126.94	115.30
1	C	68	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	198	GLY	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	2392	0	2438	53	1
1	C	2185	0	2240	62	0
2	B	2050	0	2081	39	1
2	D	2066	0	2090	40	0
3	A	27	0	22	2	0
3	C	27	0	22	5	0
4	B	6	0	7	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	6	0	7	0	0
5	A	44	0	0	2	0
5	B	37	0	0	1	0
5	C	25	0	0	2	0
5	D	28	0	0	0	0
All	All	8893	0	8907	174	1

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 10.

All (174) 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:71:HIS:HE1	2:D:304:PHE:CE2	1.66	1.13
1:C:71:HIS:CE1	2:D:304:PHE:HE2	1.65	1.12
1:C:84:HIS:CD2	1:C:296:LEU:HD13	2.01	0.96
1:A:95:ALA:O	1:A:199:ARG:NH1	2.03	0.91
1:C:212:LEU:HD11	1:C:216:PHE:CE2	2.09	0.88
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.58	0.85
2:B:323:GLN:HA	2:B:323:GLN:OE1	1.80	0.80
1:C:60:HIS:HD2	1:C:62:ASN:H	1.31	0.79
2:B:207:THR:OG1	2:B:210:MET:HG3	1.83	0.78
1:C:98:GLY:HA2	1:C:199:ARG:HD3	1.65	0.77
2:D:216:ASP:HB2	2:D:406:GLN:HG3	1.67	0.76
2:D:417:LYS:HB3	2:D:417:LYS:NZ	2.01	0.75
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.22	0.75
2:B:305:ASP:HB3	4:B:1193:SGM:H12	1.66	0.75
2:B:296:HIS:NE2	2:B:300:LYS:HE3	2.02	0.74
2:D:417:LYS:HB3	2:D:417:LYS:HZ3	1.50	0.74
1:A:177:CYS:HB2	1:A:233:MET:CE	2.19	0.73
1:C:154:VAL:O	2:D:316:THR:CG2	2.37	0.73
1:C:251:VAL:HG12	1:C:252:VAL:HG23	1.71	0.73
1:A:227:TRP:O	1:A:230:VAL:HG22	1.88	0.72
1:C:13:GLY:HA2	3:C:1297:ST8:H141	1.71	0.72
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.58	0.71
2:D:417:LYS:NZ	2:D:417:LYS:CB	2.52	0.71
1:C:213:PHE:O	1:C:217:ARG:HG3	1.91	0.69
1:A:154:VAL:O	2:B:316:THR:CG2	2.41	0.69
2:B:300:LYS:HD3	1:C:-2:PRO:O	1.92	0.69
2:B:323:GLN:OE1	2:B:324:PRO:HA	1.91	0.69
2:B:305:ASP:CB	4:B:1193:SGM:H12	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:HIS:O	1:C:122:ARG:HG3	1.95	0.68
2:B:431:ASN:OD1	2:B:431:ASN:O	2.12	0.67
1:A:260:ARG:HD3	5:A:2038:HOH:O	1.93	0.67
1:C:60:HIS:CD2	1:C:62:ASN:H	2.12	0.66
2:D:358:ALA:HB1	2:D:391:LEU:HD13	1.78	0.65
1:C:51:GLU:O	1:C:55:LEU:HB2	1.96	0.65
3:C:1297:ST8:N3	3:C:1297:ST8:H22	2.11	0.65
1:C:212:LEU:HD11	1:C:216:PHE:CZ	2.31	0.65
1:A:154:VAL:O	2:B:316:THR:HG22	1.97	0.64
2:B:310:THR:OG1	2:B:313:GLN:HG3	1.98	0.62
1:C:154:VAL:O	2:D:316:THR:HG22	2.00	0.62
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.81	0.61
3:C:1297:ST8:N3	3:C:1297:ST8:C22	2.62	0.61
2:D:417:LYS:CB	2:D:417:LYS:HZ2	2.13	0.61
1:A:295:HIS:O	1:A:296:LEU:HD23	2.01	0.60
1:A:177:CYS:HB2	1:A:233:MET:HE2	1.84	0.60
1:C:129:LYS:HD2	1:C:131:GLN:OE1	2.02	0.60
1:A:119:HIS:HD2	5:B:2003:HOH:O	1.84	0.60
2:B:296:HIS:CD2	2:B:300:LYS:HE3	2.37	0.59
1:A:291:LYS:CG	1:A:291:LYS:O	2.47	0.59
1:C:212:LEU:C	1:C:212:LEU:HD13	2.24	0.58
1:A:137:THR:O	1:A:293:VAL:HG13	2.05	0.57
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.69	0.57
1:C:291:LYS:HE3	5:C:2014:HOH:O	2.04	0.56
1:C:15:TYR:OH	1:C:51:GLU:OE1	2.22	0.56
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.40	0.56
2:D:383:THR:OG1	2:D:385:GLU:HB3	2.06	0.56
3:A:1298:ST8:N3	3:A:1298:ST8:C22	2.68	0.56
2:B:293:ARG:HD3	1:C:2:GLU:OE1	2.05	0.56
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.88	0.56
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.88	0.55
3:A:1298:ST8:N3	3:A:1298:ST8:H22	2.21	0.55
1:A:72:THR:O	2:B:296:HIS:HE1	1.89	0.55
1:A:92:ASP:O	1:A:95:ALA:HB2	2.07	0.55
1:A:252:VAL:HG11	1:A:255:LEU:HD22	1.87	0.55
1:A:71:HIS:CD2	2:B:296:HIS:CE1	2.94	0.54
1:C:12:GLU:HG2	1:C:17:VAL:HG13	1.88	0.54
1:C:212:LEU:CD1	1:C:216:PHE:CE2	2.87	0.54
2:B:305:ASP:HB3	4:B:1193:SGM:C1	2.35	0.54
1:A:51:GLU:O	1:A:55:LEU:HB2	2.08	0.53
1:C:15:TYR:HE2	1:C:35:ILE:HG12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:LEU:HD23	1:C:136:ASN:HB3	1.89	0.53
2:D:346:PRO:O	2:D:349:LYS:HG2	2.08	0.53
2:D:412:LYS:HD3	2:D:413:TYR:CE1	2.44	0.52
2:D:337:GLY:O	2:D:340:SER:OG	2.19	0.52
1:A:115:LEU:HD21	1:A:185:ASP:HB3	1.91	0.52
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.45	0.52
1:A:162:GLU:H	1:A:162:GLU:CD	2.13	0.52
2:D:395:HIS:HE1	2:D:427:PRO:O	1.92	0.52
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.46	0.51
2:D:262:LEU:HD11	2:D:266:LYS:HE3	1.94	0.50
1:A:71:HIS:CE1	2:B:296:HIS:CD2	3.00	0.50
1:C:38:ASP:HB3	1:C:41:THR:HB	1.94	0.50
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.47	0.49
1:A:278:LYS:NZ	2:B:181:ASP:OD2	2.45	0.49
1:C:87:LEU:O	1:C:91:MET:HG3	2.11	0.49
1:C:15:TYR:CE2	1:C:35:ILE:HG12	2.48	0.49
1:C:210:ASP:O	1:C:214:ARG:HG3	2.12	0.49
2:D:314:PHE:O	2:D:315:LEU:C	2.49	0.49
1:C:85:GLN:OE1	1:C:89:LYS:HD3	2.13	0.48
1:A:73:GLU:OE2	1:C:2:GLU:OE2	2.31	0.48
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.95	0.48
1:A:89:LYS:NZ	1:A:297:ARG:HH12	2.11	0.48
1:A:20:LYS:HE3	1:A:29:VAL:HG11	1.96	0.47
2:D:371:SER:O	2:D:372:TRP:C	2.52	0.47
2:B:211:ARG:HD3	2:B:344:ALA:HB2	1.95	0.47
1:C:71:HIS:CE1	2:D:304:PHE:CE2	2.58	0.47
1:A:230:VAL:O	1:A:233:MET:HG3	2.15	0.47
1:C:248:PHE:O	1:C:251:VAL:HB	2.15	0.47
1:A:71:HIS:NE2	2:B:296:HIS:NE2	2.62	0.46
2:D:215:VAL:O	2:D:219:VAL:HG23	2.15	0.46
1:C:84:HIS:HD2	1:C:296:LEU:HD13	1.70	0.46
1:C:249:SER:HA	1:C:260:ARG:HD2	1.97	0.46
2:B:300:LYS:NZ	1:C:0:SER:OG	2.44	0.46
1:C:10:ILE:CG2	3:C:1297:ST8:H101	2.46	0.46
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.45	0.46
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.50	0.46
2:D:323:GLN:HA	2:D:324:PRO:HA	1.78	0.46
2:D:417:LYS:HZ2	2:D:417:LYS:HB2	1.81	0.46
2:B:190:GLU:HG3	2:B:351:LEU:HD22	1.98	0.46
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.50	0.46
5:A:2006:HOH:O	2:B:316:THR:HG21	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:HB2	1:C:269:TYR:OH	2.16	0.45
1:A:35:ILE:HB	1:A:76:LEU:HB3	1.99	0.45
1:C:120:SER:HB3	1:C:121:HIS:ND1	2.31	0.45
1:A:223:ASP:H	1:A:226:VAL:HG12	1.81	0.45
1:A:223:ASP:OD1	1:A:226:VAL:HG12	2.17	0.45
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.81	0.45
1:C:120:SER:HB3	1:C:121:HIS:HD1	1.82	0.45
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.81	0.45
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.98	0.45
1:A:119:HIS:CD2	1:A:182:THR:HB	2.51	0.45
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.64	0.45
1:A:294:PRO:C	1:A:296:LEU:H	2.20	0.45
2:B:417:LYS:NZ	2:B:417:LYS:CB	2.80	0.45
1:A:256:ASP:O	1:A:260:ARG:HG3	2.16	0.45
1:C:88:LYS:HD3	1:C:131:GLN:NE2	2.32	0.44
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.52	0.44
2:B:199:TYR:CE1	2:B:243:LEU:HB3	2.52	0.44
1:C:72:THR:HG22	1:C:73:GLU:H	1.83	0.44
2:D:372:TRP:HB3	2:D:384:LEU:HD13	2.00	0.44
2:D:344:ALA:HB1	2:D:348:LEU:HD22	2.00	0.44
2:D:344:ALA:O	2:D:348:LEU:HB2	2.17	0.44
1:C:72:THR:HG22	1:C:73:GLU:N	2.32	0.44
1:C:154:VAL:O	2:D:316:THR:HG23	2.17	0.44
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.99	0.44
2:D:216:ASP:CB	2:D:406:GLN:HG3	2.41	0.44
1:C:81:GLU:O	1:C:81:GLU:HG3	2.18	0.44
2:D:315:LEU:HD23	2:D:315:LEU:HA	1.79	0.44
1:A:3:ASN:O	1:A:24:LYS:HG3	2.18	0.44
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.64	0.44
1:C:13:GLY:CA	3:C:1297:ST8:H141	2.46	0.43
1:C:57:GLU:OE2	2:D:307:ALA:HB3	2.17	0.43
1:A:15:TYR:HE2	1:A:35:ILE:HG12	1.83	0.43
1:A:71:HIS:CE1	2:B:296:HIS:NE2	2.87	0.43
1:C:203:PHE:HB2	1:C:211:GLN:HE22	1.84	0.43
1:A:155:PRO:HD2	2:B:316:THR:HG23	2.00	0.43
2:D:223:GLU:OE2	2:D:412:LYS:HE3	2.19	0.43
2:D:207:THR:OG1	2:D:210:MET:HG3	2.19	0.42
2:D:255:LEU:HD11	2:D:291:VAL:HA	2.01	0.42
1:C:119:HIS:CD2	1:C:182:THR:HB	2.55	0.42
1:A:2:GLU:HG2	2:D:293:ARG:HH12	1.85	0.42
2:B:345:ASP:HA	2:B:346:PRO:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:PHE:HA	2:B:281:ILE:HG12	2.01	0.42
1:C:41:THR:HB	1:C:42:GLU:H	1.63	0.42
1:A:42:GLU:HA	2:B:275:VAL:HG21	2.02	0.42
2:D:391:LEU:HD13	2:D:391:LEU:HA	1.91	0.42
2:B:218:LEU:HD23	2:B:218:LEU:HA	1.95	0.41
1:A:133:LEU:HD11	1:A:192:ILE:HD13	2.01	0.41
2:B:323:GLN:HA	2:B:324:PRO:HA	1.78	0.41
1:A:217:ARG:HG2	1:A:243:TRP:CE2	2.55	0.41
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.85	0.41
1:A:290:THR:HG23	1:A:292:PRO:HD3	2.02	0.41
1:A:231:THR:HA	1:A:236:TYR:CD1	2.56	0.41
2:D:345:ASP:HA	2:D:346:PRO:HA	1.78	0.41
1:A:250:LYS:HA	1:A:250:LYS:HD3	1.87	0.41
2:B:217:TRP:CZ2	2:B:281:ILE:HD12	2.55	0.41
1:C:3:ASN:O	1:C:24:LYS:HG3	2.20	0.41
1:A:110:GLN:OE1	1:A:140:ALA:HA	2.21	0.41
1:C:2:GLU:O	1:C:24:LYS:HE3	2.20	0.41
1:C:65:LYS:HG2	5:C:2008:HOH:O	2.21	0.41
2:B:388:LYS:O	2:B:389:PRO:C	2.59	0.41
1:C:121:HIS:C	1:C:122:ARG:HG3	2.41	0.40
1:A:252:VAL:CG1	1:A:255:LEU:HD22	2.50	0.40
2:B:376:LEU:HA	2:B:376:LEU:HD23	1.83	0.40
1:A:227:TRP:CE3	1:A:269:TYR:HB3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:NH2	2:B:374:GLU:OE2[4_456]	2.07	0.13

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/302 (97%)	281 (96%)	10 (3%)	2 (1%)	22	43
1	C	268/302 (89%)	250 (93%)	12 (4%)	6 (2%)	6	12
2	B	250/260 (96%)	245 (98%)	5 (2%)	0	100	100
2	D	254/260 (98%)	242 (95%)	12 (5%)	0	100	100
All	All	1065/1124 (95%)	1018 (96%)	39 (4%)	8 (1%)	19	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	A	164	VAL
1	A	295	HIS
1	C	145	ASP
1	C	162	GLU
1	C	40	GLU
1	C	251	VAL
1	C	166	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/264 (99%)	237 (91%)	24 (9%)	9	17
1	C	238/264 (90%)	215 (90%)	23 (10%)	8	15
2	B	228/234 (97%)	216 (95%)	12 (5%)	22	45
2	D	230/234 (98%)	211 (92%)	19 (8%)	11	22
All	All	957/996 (96%)	879 (92%)	78 (8%)	11	22

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	ARG
1	A	41	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	49	ILE
1	A	55	LEU
1	A	59	ASN
1	A	73	GLU
1	A	74	ASN
1	A	75	LYS
1	A	83	LEU
1	A	101	LEU
1	A	120	SER
1	A	122	ARG
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	178	LYS
1	A	181	SER
1	A	206	ASP
1	A	230	VAL
1	A	248	PHE
1	A	255	LEU
1	A	278	LYS
2	B	209	SER
2	B	232	LEU
2	B	292	LEU
2	B	316	THR
2	B	323	GLN
2	B	348	LEU
2	B	371	SER
2	B	384	LEU
2	B	391	LEU
2	B	392	MET
2	B	398	TYR
2	B	417	LYS
1	C	9	LYS
1	C	17	VAL
1	C	34	LYS
1	C	41	THR
1	C	56	LYS
1	C	75	LYS
1	C	83	LEU
1	C	96	LEU
1	C	101	LEU

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Mol	Chain	Res	Type
1	C	120	SER
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG
1	C	157	ARG
1	C	163	VAL
1	C	178	LYS
1	C	200	ARG
1	C	206	ASP
1	C	217	ARG
1	C	248	PHE
1	C	250	LYS
1	C	278	LYS
1	C	295	HIS
2	D	196	LYS
2	D	199	TYR
2	D	205	ASP
2	D	223	GLU
2	D	232	LEU
2	D	247	SER
2	D	250	ARG
2	D	284	ASP
2	D	292	LEU
2	D	293	ARG
2	D	313	GLN
2	D	316	THR
2	D	348	LEU
2	D	386	SER
2	D	391	LEU
2	D	398	TYR
2	D	417	LYS
2	D	424	LEU
2	D	429	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	295	HIS
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN

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Mol	Chain	Res	Type
2	B	395	HIS
2	B	396	GLN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	113	GLN
1	C	119	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	395	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	C	160	1	8,10,11	1.34	1 (12%)	10,14,16	1.18	1 (10%)
1	TPO	A	160	1	8,10,11	1.60	1 (12%)	10,14,16	1.15	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	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-OG1	-3.74	1.52	1.59
1	C	160	TPO	P-OG1	-3.43	1.52	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-2.67	117.78	124.78
1	A	160	TPO	O-C-CA	-2.18	119.06	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	ST8	C	1297	-	29,29,29	1.43	4 (13%)	39,39,39	2.06	12 (30%)
4	SGM	D	1193	2	5,5,5	1.50	1 (20%)	5,5,5	1.30	1 (20%)
3	ST8	A	1298	-	29,29,29	1.35	3 (10%)	39,39,39	1.91	12 (30%)
4	SGM	B	1193	2	5,5,5	0.65	0	5,5,5	0.38	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ST8	C	1297	-	-	3/15/23/23	0/3/3/3
4	SGM	D	1193	2	-	2/4/4/4	-
3	ST8	A	1298	-	-	0/15/23/23	0/3/3/3
4	SGM	B	1193	2	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1297	ST8	C23-N25	5.40	1.43	1.33
3	A	1298	ST8	C23-N25	5.08	1.42	1.33
4	D	1193	SGM	C1-S1	-3.24	1.74	1.81
3	C	1297	ST8	C4-N3	2.58	1.36	1.32
3	A	1298	ST8	C5-C6	2.50	1.48	1.41
3	A	1298	ST8	C5-C4	2.29	1.46	1.41
3	C	1297	ST8	C5-C6	2.12	1.47	1.41
3	C	1297	ST8	C5-C4	2.03	1.45	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	ST8	C20-C23-N25	5.86	124.78	117.75
3	C	1297	ST8	C6-C5-C4	4.85	117.79	114.57
3	C	1297	ST8	C15-C16-C11	-4.69	103.28	112.15
3	C	1297	ST8	C2-N3-C4	4.26	122.80	115.18
3	C	1297	ST8	C5-C4-N3	-4.11	117.74	123.46
3	A	1298	ST8	C2-N3-C4	3.90	122.17	115.18
3	C	1297	ST8	N1-C2-N3	-3.47	120.75	126.23
3	A	1298	ST8	C5-C4-N3	-3.41	118.71	123.46
3	A	1298	ST8	O24-C23-N25	-3.29	117.90	122.58
3	C	1297	ST8	C13-C12-C11	-3.23	106.05	112.15
3	A	1298	ST8	C13-C12-C11	-3.18	106.14	112.15
3	C	1297	ST8	C2-N1-C6	2.87	122.41	116.52
3	A	1298	ST8	C6-C5-C4	2.86	116.47	114.57
3	C	1297	ST8	C20-C23-N25	2.80	121.11	117.75
3	C	1297	ST8	C17-N2-C2	-2.70	121.41	129.23
3	A	1298	ST8	O6-C4-C5	2.68	119.97	116.57
3	A	1298	ST8	C15-C16-C11	-2.68	107.08	112.15
3	C	1297	ST8	C10-O6-C4	-2.66	114.96	117.50
4	D	1193	SGM	C2-C1-S1	-2.54	107.09	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297	ST8	N9-C6-N1	2.50	120.57	117.03
3	C	1297	ST8	O24-C23-N25	-2.22	119.42	122.58
3	A	1298	ST8	N9-C6-N1	2.13	120.05	117.03
3	A	1298	ST8	C17-N2-C2	-2.11	123.11	129.23
3	A	1298	ST8	O24-C23-C20	-2.03	117.20	119.63
3	A	1298	ST8	C2-N1-C6	2.01	120.64	116.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

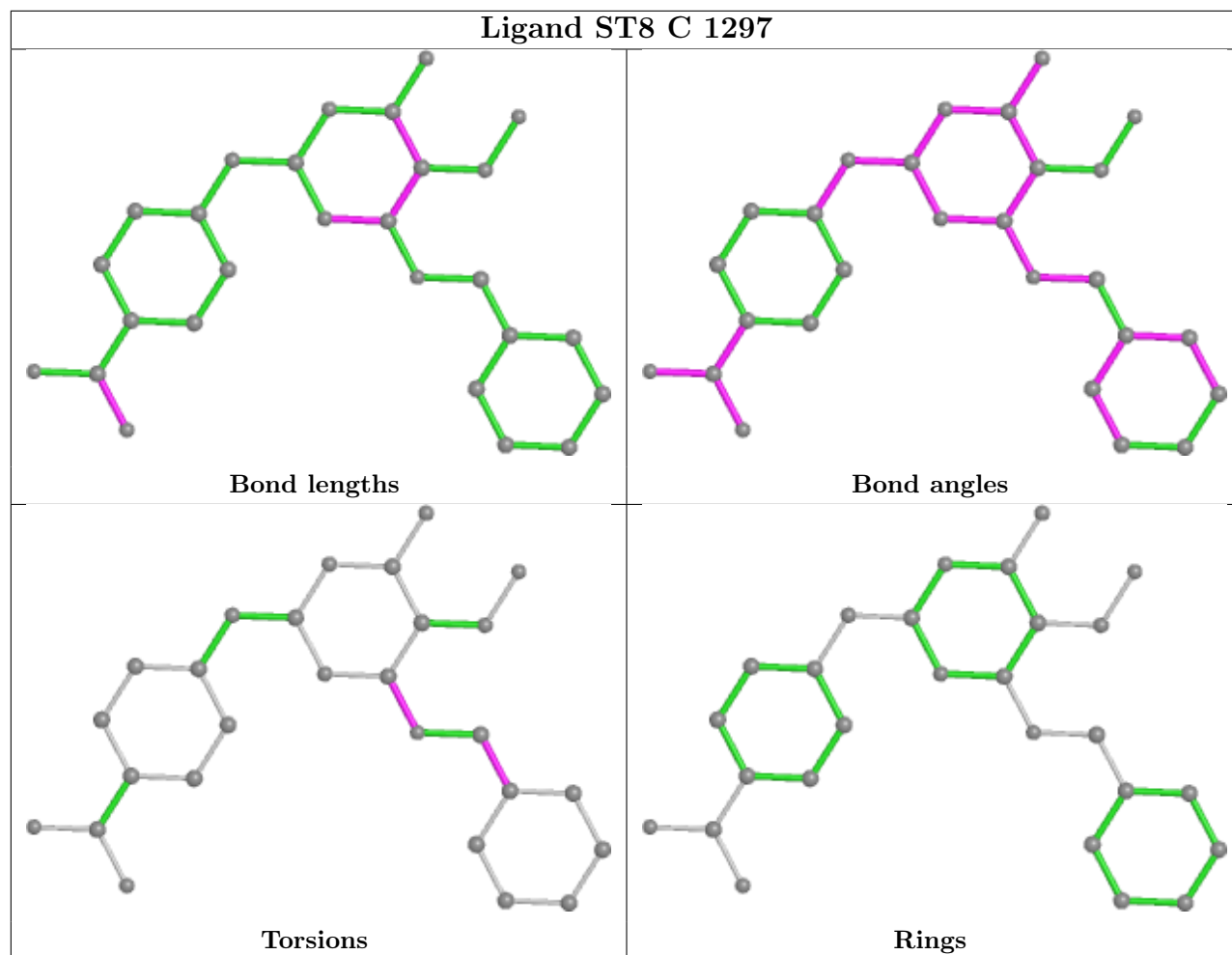
Mol	Chain	Res	Type	Atoms
3	C	1297	ST8	O6-C10-C11-C12
4	D	1193	SGM	C1-C2-C3-O3
3	C	1297	ST8	O6-C10-C11-C16
4	D	1193	SGM	O2-C2-C3-O3
3	C	1297	ST8	N3-C4-O6-C10

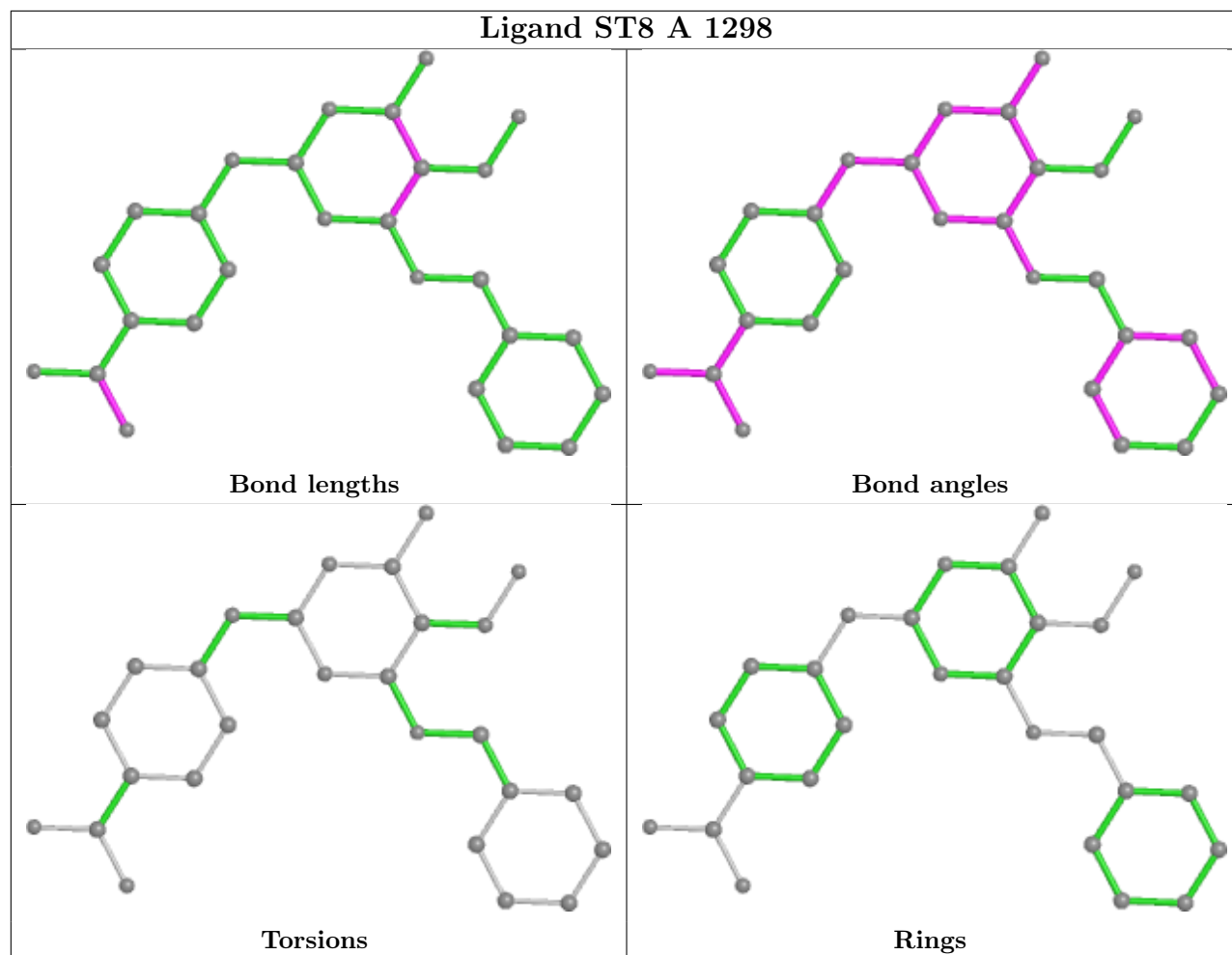
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	ST8	5	0
3	A	1298	ST8	2	0
4	B	1193	SGM	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/302 (98%)	-0.40	5 (1%) 70 66	13, 23, 43, 62	0
1	C	272/302 (90%)	-0.02	10 (3%) 41 34	22, 37, 57, 75	0
2	B	253/260 (97%)	-0.44	5 (1%) 65 60	14, 26, 44, 58	0
2	D	255/260 (98%)	0.04	9 (3%) 44 36	20, 38, 61, 75	0
All	All	1076/1124 (95%)	-0.21	29 (2%) 54 48	13, 31, 56, 75	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	5.1
1	C	293	VAL	4.0
1	C	250	LYS	3.6
2	D	428	GLU	3.6
1	A	95	ALA	3.4
1	C	295	HIS	3.4
2	D	324	PRO	3.3
2	B	323	GLN	3.2
2	D	432	LEU	3.1
1	C	249	SER	3.1
2	D	325	ALA	2.9
2	D	311	VAL	2.8
1	C	221	THR	2.8
1	C	96	LEU	2.7
2	B	431	ASN	2.7
1	A	73	GLU	2.7
2	D	431	ASN	2.6
2	D	284	ASP	2.5
1	C	273	LYS	2.5
2	D	283	ASP	2.5
1	C	256	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	2.4
2	B	324	PRO	2.4
1	A	71	HIS	2.4
1	C	162	GLU	2.2
2	B	201	LYS	2.2
1	C	296	LEU	2.2
2	B	432	LEU	2.1
2	D	323	GLN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TPO	C	160	11/12	0.97	0.14	28,34,40,40	0
1	TPO	A	160	11/12	0.99	0.10	18,22,24,25	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

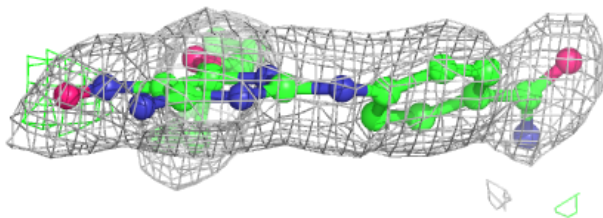
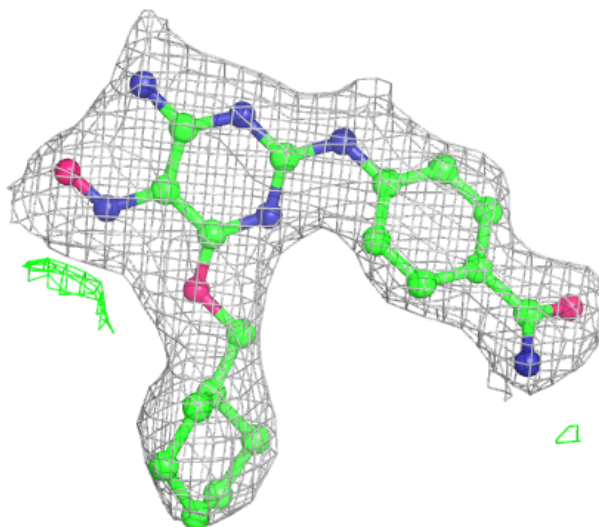
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

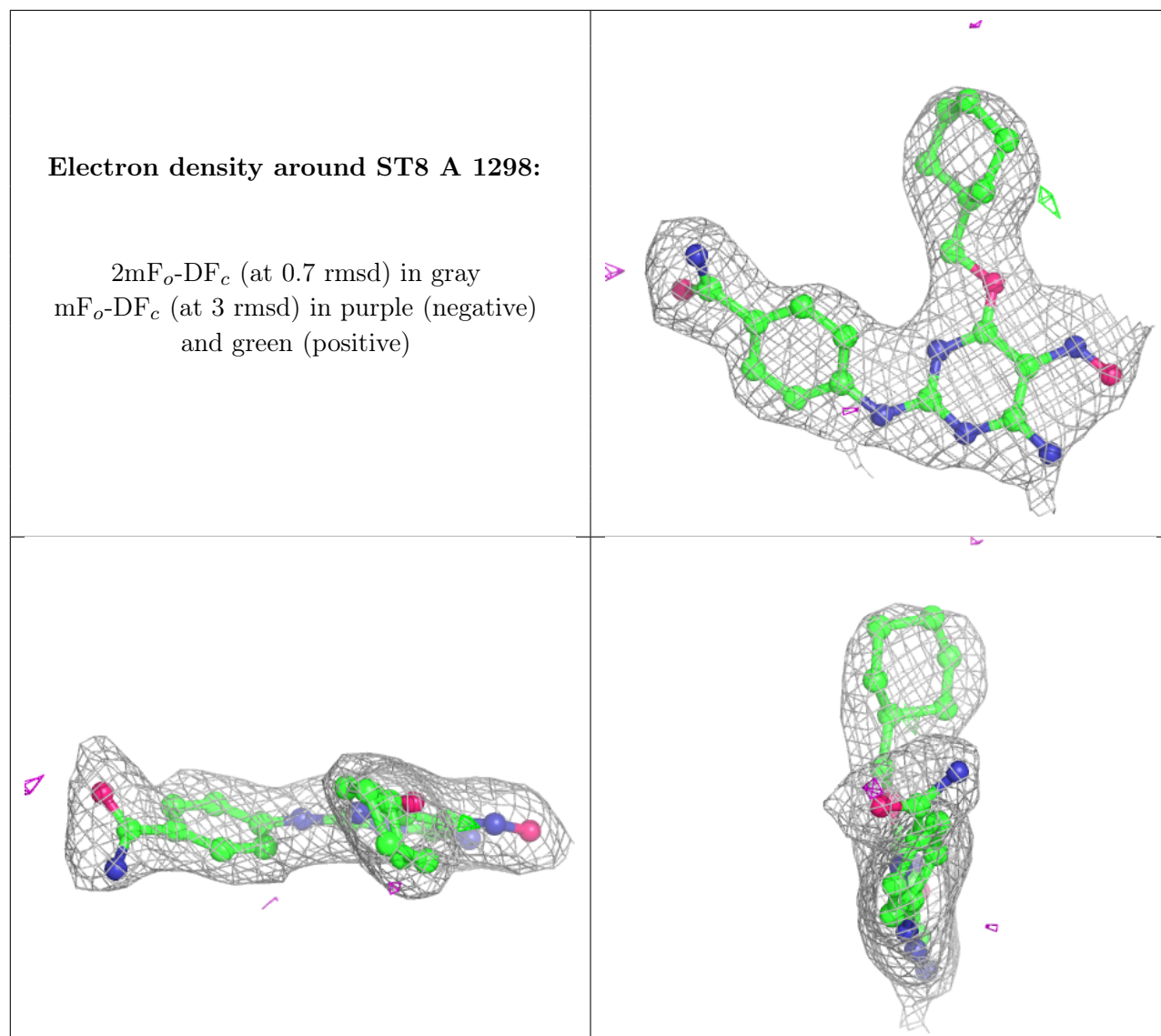
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ST8	C	1297	27/27	0.93	0.16	26,30,39,40	0
3	ST8	A	1298	27/27	0.95	0.14	24,29,37,38	0
4	SGM	B	1193	6/6	0.95	0.15	30,33,37,45	0
4	SGM	D	1193	6/6	0.95	0.14	45,47,48,48	0

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 ST8 C 1297:**

$2mF_o-DF_c$  (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.