Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 05:45 am BST

PDB ID	:	4BCM
Title	:	Structure of CDK2 in complex with cyclin A and a 2-amino-4-heteroaryl-pyrimidine inhibitor
Authors	:	Hole, A.J.; Baumli, S.; Wang, S.; Endicott, J.A.; Noble, M.E.M.
Deposited on	:	2012-10-02
Resolution	:	2.45 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 following versions of software and data (see references (i)) were used in the production of this report:

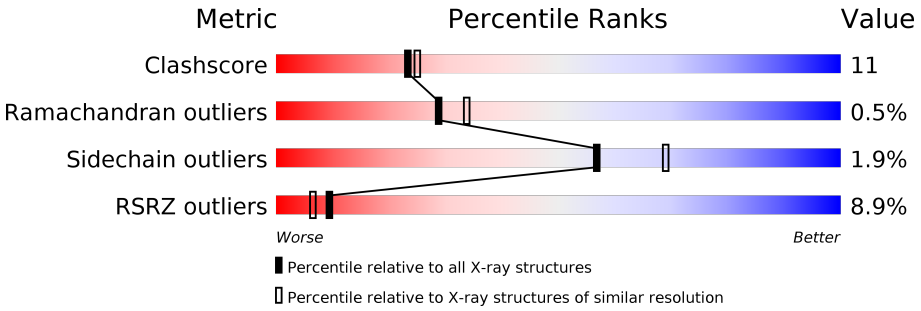
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

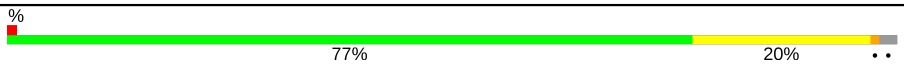
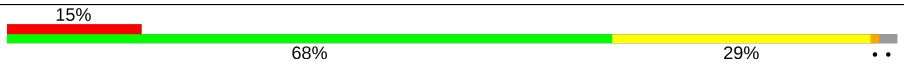
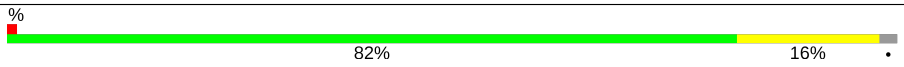
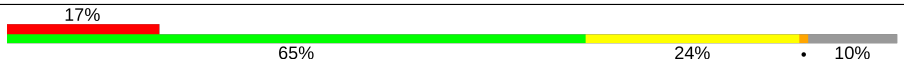
The reported resolution of this entry is 2.45 Å.

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))
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	301	
1	C	301	
2	B	262	
3	D	262	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYCLIN-DEPENDENT KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	0	0
			2375	1544	403	419	1	8			
1	C	295	Total	C	N	O	P	S	0	0	0
			2370	1538	400	423	1	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	1	0
			2083	1350	340	382	11			

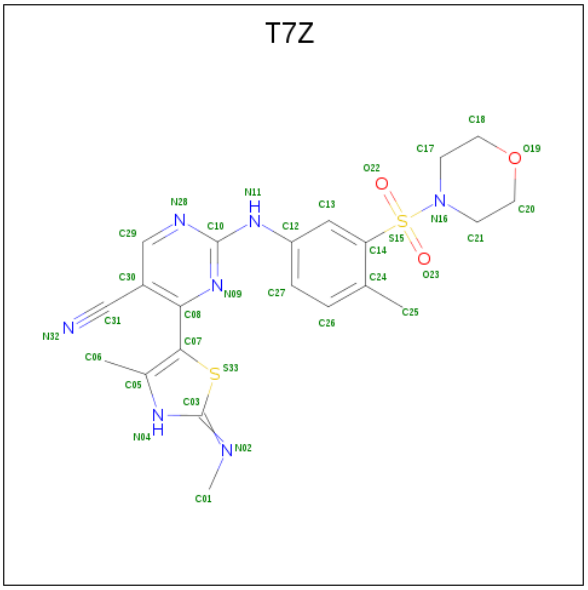
- Molecule 3 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	236	Total	C	N	O	S	0	0	0
			1918	1249	311	348	10			

There is a discrepancy between the modelled and reference sequences:

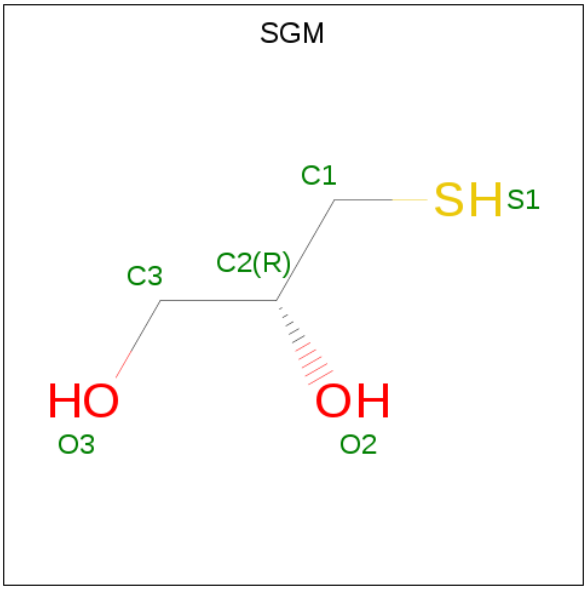
Chain	Residue	Modelled	Actual	Comment	Reference
D	331	LEU	SER	conflict	UNP P20248

- Molecule 4 is 4-(4-methyl-2-methylimino-3H-1,3-thiazol-5-yl)-2-[(4-methyl-3-morpholin-4-ylsulfonyl-phenyl)amino]pyrimidine-5-carbonitrile (three-letter code: T7Z) (formula: $C_{21}H_{23}N_7O_3S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			33	21	7	3	2		
4	C	1	Total	C	N	O	S	0	0
			33	21	7	3	2		

- Molecule 5 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



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

- Molecule 6 is water.

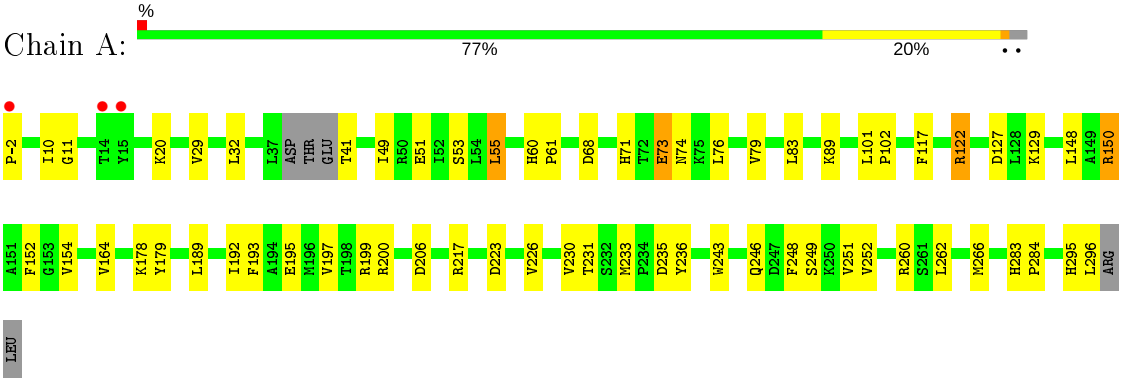
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	106	Total	O	0	0
			106	106		
6	C	36	Total	O	0	0
			36	36		
6	D	17	Total	O	0	0
			17	17		

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.

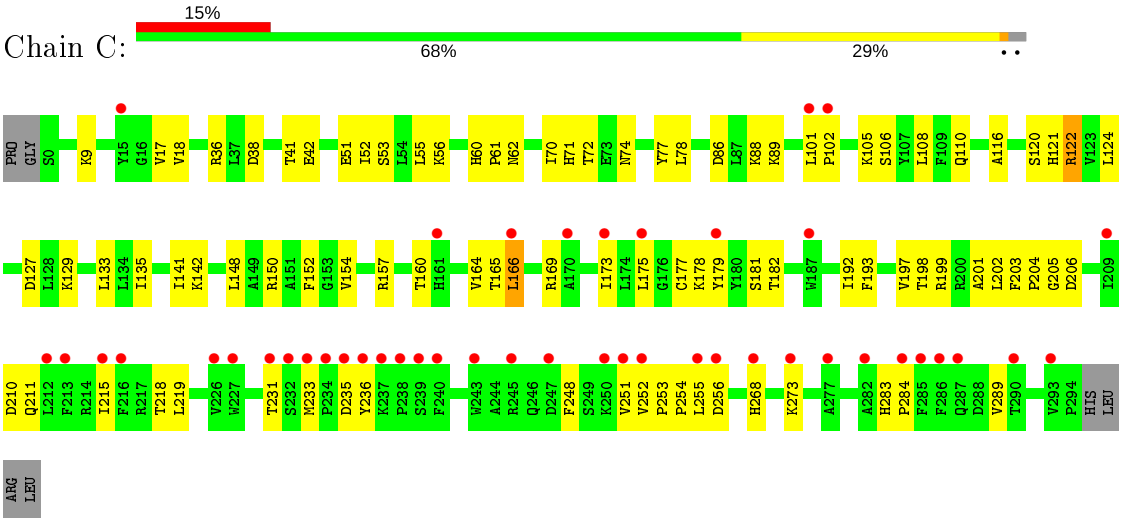
- Molecule 1: CYCLIN-DEPENDENT KINASE 2

Chain A:



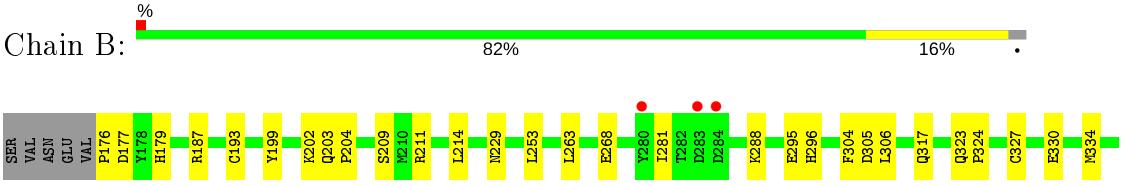
- Molecule 1: CYCLIN-DEPENDENT KINASE 2

Chain C:



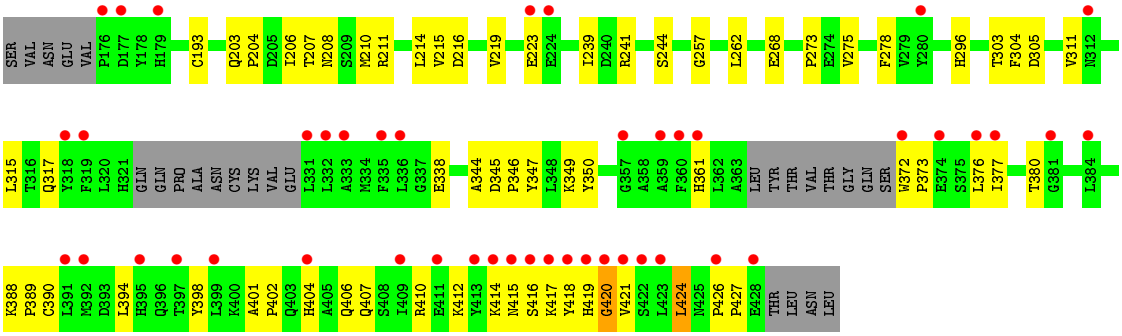
- Molecule 2: CYCLIN-A2

Chain B:



- Molecule 3: 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	74.07Å 135.41Å 148.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.46 – 2.45 52.46 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (52.46-2.45) 99.0 (52.46-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.196 , 0.258 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9111	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, T7Z, SGM

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	0.38	0/2425	0.56	0/3288
1	C	0.29	0/2419	0.46	0/3282
2	B	0.37	0/2137	0.51	0/2901
3	D	0.29	0/1964	0.45	0/2661
All	All	0.34	0/8945	0.50	0/12132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2375	0	2422	52	0
1	C	2370	0	2412	66	0
2	B	2083	0	2105	38	0
3	D	1918	0	1941	54	0
4	A	33	0	23	8	0
4	C	33	0	23	4	0
5	B	6	0	7	2	0
5	D	6	0	7	2	0
6	A	128	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	106	0	0	4	0
6	C	36	0	0	3	0
6	D	17	0	0	1	0
All	All	9111	0	8940	200	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 11.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:CYS:SG	5:B:1433:SGM:S1	2.29	1.30
3:D:193:CYS:SG	5:D:1429:SGM:S1	2.31	1.28
3:D:305:ASP:HB3	5:D:1429:SGM:H12	1.55	0.85
1:C:72:THR:HG22	1:C:74:ASN:H	1.48	0.78
1:A:-2:PRO:HA	1:A:68:ASP:OD2	1.83	0.77
1:A:89:LYS:NZ	4:A:1297:T7Z:H172	2.01	0.75
4:C:1295:T7Z:H061	4:C:1295:T7Z:C31	2.15	0.75
1:A:223:ASP:OD1	1:A:226:VAL:HG12	1.86	0.75
1:A:51:GLU:O	1:A:55:LEU:HB2	1.89	0.73
1:A:150:ARG:NH2	2:B:268:GLU:O	2.20	0.73
2:B:327:CYS:SG	6:B:2073:HOH:O	2.45	0.73
2:B:317:GLN:OE1	6:B:2016:HOH:O	2.06	0.73
2:B:305:ASP:HB3	5:B:1433:SGM:H12	1.71	0.72
4:A:1297:T7Z:C31	4:A:1297:T7Z:H061	2.21	0.68
1:A:73:GLU:HG2	1:A:74:ASN:N	2.08	0.68
1:C:268:HIS:CE1	1:C:273:LYS:HD2	2.28	0.68
1:C:204:PRO:O	6:C:2034:HOH:O	2.12	0.68
3:D:303:THR:HG22	3:D:303:THR:O	1.93	0.68
1:C:251:VAL:HG12	1:C:252:VAL:HG23	1.75	0.68
1:C:157:ARG:O	6:C:2024:HOH:O	2.11	0.68
1:A:89:LYS:HZ3	4:A:1297:T7Z:H172	1.60	0.67
1:A:246:GLN:NE2	6:A:2107:HOH:O	2.25	0.67
2:B:203:GLN:O	6:B:2025:HOH:O	2.12	0.65
3:D:346:PRO:O	3:D:349:LYS:HG2	1.98	0.64
1:C:52:ILE:O	1:C:56:LYS:HG3	1.97	0.64
3:D:417:LYS:HD3	3:D:418:TYR:CZ	2.33	0.63
1:C:197:VAL:HG23	1:C:198:THR:HG23	1.78	0.63
3:D:401:ALA:HB3	3:D:402:PRO:HD3	1.81	0.63
3:D:407:GLN:OE1	3:D:410:ARG:HD3	1.99	0.62
1:C:121:HIS:O	1:C:122:ARG:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:ND1	1:C:61:PRO:HD2	2.15	0.62
1:C:51:GLU:O	1:C:55:LEU:HB2	2.00	0.61
1:C:86:ASP:OD1	1:C:89:LYS:HG2	2.00	0.61
1:A:51:GLU:OE2	6:A:2016:HOH:O	2.16	0.61
3:D:303:THR:CG2	3:D:303:THR:O	2.49	0.60
1:C:105:LYS:HG2	1:C:289:VAL:HG23	1.83	0.60
3:D:346:PRO:HB2	3:D:349:LYS:HE2	1.84	0.60
1:C:177:CYS:HB2	1:C:233:MET:SD	2.43	0.59
3:D:216:ASP:O	3:D:219:VAL:HB	2.02	0.59
1:A:60:HIS:ND1	1:A:61:PRO:HD2	2.18	0.59
1:A:73:GLU:HG2	1:A:74:ASN:H	1.68	0.59
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.38	0.59
3:D:203:GLN:O	6:D:2002:HOH:O	2.17	0.58
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.38	0.58
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.84	0.58
1:C:231:THR:HG23	1:C:236:TYR:CE1	2.38	0.58
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.39	0.58
1:A:71:HIS:NE2	2:B:296:HIS:NE2	2.52	0.57
1:C:178:LYS:HE2	1:C:179:TYR:HE2	1.69	0.57
2:B:263:LEU:HD21	2:B:295:GLU:HG3	1.88	0.56
1:C:165:THR:HG22	6:C:2028:HOH:O	2.05	0.56
3:D:372:TRP:NE1	3:D:377:ILE:HG12	2.21	0.55
1:A:223:ASP:H	1:A:226:VAL:CG1	2.19	0.55
1:C:60:HIS:CE1	1:C:61:PRO:HD2	2.41	0.55
1:C:201:ALA:HB3	1:C:204:PRO:HG3	1.88	0.55
1:C:121:HIS:C	1:C:122:ARG:HG3	2.27	0.55
1:C:205:GLY:HA3	1:C:211:GLN:OE1	2.06	0.55
1:C:253:PRO:HD2	1:C:254:PRO:HD2	1.87	0.55
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.42	0.55
4:A:1297:T7Z:C31	4:A:1297:T7Z:C06	2.85	0.54
4:C:1295:T7Z:C06	4:C:1295:T7Z:C31	2.86	0.54
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.44	0.53
1:A:127:ASP:HB2	1:A:148:LEU:HD12	1.91	0.52
2:B:176:PRO:HA	2:B:179[B]:HIS:CG	2.45	0.52
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.91	0.51
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.75	0.51
1:C:116:ALA:O	1:C:120:SER:OG	2.22	0.51
1:C:203:PHE:CE1	1:C:215:ILE:HA	2.46	0.51
3:D:303:THR:O	3:D:304:PHE:HB2	2.10	0.51
2:B:187:ARG:HD3	6:B:2019:HOH:O	2.10	0.51
1:C:18:VAL:HG21	4:C:1295:T7Z:N04	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ILE:HG22	1:C:141:ILE:HG13	1.93	0.51
1:A:41:THR:O	2:B:288:LYS:NZ	2.28	0.51
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.25	0.51
1:C:178:LYS:HE2	1:C:179:TYR:CE2	2.46	0.51
3:D:216:ASP:CG	3:D:406:GLN:HB3	2.31	0.51
2:B:176:PRO:HA	2:B:179[B]:HIS:CE1	2.47	0.50
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.93	0.50
2:B:346:PRO:HD2	2:B:347:TYR:CD2	2.47	0.49
3:D:376:LEU:O	3:D:380:THR:HG23	2.12	0.49
3:D:419:HIS:N	3:D:419:HIS:CD2	2.80	0.49
3:D:402:PRO:HA	3:D:410:ARG:NH1	2.28	0.49
1:C:197:VAL:HG21	1:C:252:VAL:CG1	2.43	0.49
1:C:206:ASP:HB2	1:C:210:ASP:OD2	2.12	0.49
1:A:10:ILE:CG2	4:A:1297:T7Z:H211	2.43	0.49
1:C:106:SER:O	1:C:110:GLN:HG3	2.13	0.48
3:D:216:ASP:OD1	3:D:406:GLN:HB3	2.13	0.48
3:D:347:TYR:OH	3:D:394:LEU:HA	2.13	0.48
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.94	0.48
3:D:203:GLN:HB3	3:D:206:ILE:HG12	1.95	0.48
3:D:388:LYS:HB3	3:D:389:PRO:HD3	1.95	0.48
1:A:20:LYS:HE3	1:A:29:VAL:HG11	1.96	0.48
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.49	0.48
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.81	0.48
1:C:253:PRO:CD	1:C:254:PRO:HD2	2.43	0.47
1:C:42:GLU:OE1	3:D:275:VAL:HG23	2.13	0.47
1:A:60:HIS:CE1	1:A:61:PRO:HD2	2.49	0.47
3:D:211:ARG:O	3:D:215:VAL:HG23	2.14	0.47
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.97	0.47
1:C:56:LYS:NZ	3:D:303:THR:HG22	2.30	0.47
1:C:154:VAL:HB	3:D:317:GLN:HG2	1.97	0.47
3:D:215:VAL:O	3:D:219:VAL:HG23	2.14	0.47
1:A:262:LEU:O	1:A:266:MET:HG3	2.14	0.47
3:D:424:LEU:HD23	3:D:424:LEU:N	2.29	0.47
2:B:176:PRO:HA	2:B:179[B]:HIS:ND1	2.30	0.47
3:D:345:ASP:HA	3:D:346:PRO:HA	1.66	0.47
1:A:235:ASP:O	6:A:2099:HOH:O	2.20	0.47
3:D:241:ARG:O	3:D:244:SER:HB2	2.15	0.47
1:A:89:LYS:HZ1	4:A:1297:T7Z:H172	1.77	0.47
1:C:197:VAL:HG23	1:C:198:THR:N	2.30	0.47
1:A:127:ASP:CG	1:A:148:LEU:HD12	2.36	0.46
2:B:229:ASN:HD22	2:B:334:MET:CE	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:214:LEU:HD21	3:D:239:ILE:HD13	1.97	0.46
1:A:249:SER:HA	1:A:260:ARG:HD3	1.98	0.46
3:D:404:HIS:CD2	3:D:406:GLN:H	2.34	0.46
3:D:421:VAL:O	3:D:424:LEU:HG	2.16	0.46
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.84	0.45
3:D:361:HIS:HD1	3:D:372:TRP:N	2.15	0.45
1:C:215:ILE:CG2	1:C:219:LEU:HD12	2.47	0.45
1:C:202:LEU:HG	1:C:203:PHE:CE2	2.51	0.45
2:B:346:PRO:HB2	2:B:349:LYS:HE2	1.98	0.45
3:D:404:HIS:NE2	3:D:406:GLN:HG2	2.31	0.45
3:D:273:PRO:HB2	3:D:278:PHE:CE2	2.52	0.45
3:D:208:ASN:OD1	3:D:344:ALA:HB3	2.17	0.45
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.05	0.44
1:C:101:LEU:N	1:C:102:PRO:CD	2.80	0.44
1:C:71:HIS:CE1	3:D:296:HIS:HE2	2.34	0.44
1:C:169:ARG:HG3	1:C:173:ILE:HD12	1.97	0.44
1:C:53:SER:HB3	3:D:304:PHE:O	2.17	0.44
1:C:86:ASP:HA	1:C:133:LEU:O	2.17	0.44
3:D:203:GLN:HB3	3:D:206:ILE:CG1	2.48	0.44
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.47	0.44
2:B:330:GLU:O	2:B:334:MET:HG2	2.17	0.44
1:C:175:LEU:O	1:C:235:ASP:HB2	2.18	0.44
1:A:154:VAL:HG13	2:B:179[B]:HIS:CD2	2.53	0.44
1:A:127:ASP:CB	1:A:148:LEU:HD12	2.48	0.44
2:B:281:ILE:H	2:B:281:ILE:HG13	1.66	0.44
1:C:150:ARG:NH1	1:C:160:TPO:O2P	2.45	0.44
3:D:426:PRO:HA	3:D:427:PRO:HD3	1.78	0.44
1:C:197:VAL:HG21	1:C:252:VAL:HG11	1.99	0.44
3:D:372:TRP:HE1	3:D:377:ILE:HG12	1.83	0.44
1:C:253:PRO:N	1:C:254:PRO:HD2	2.33	0.43
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.53	0.43
1:C:9:LYS:HE3	1:C:17:VAL:CG1	2.48	0.43
3:D:350:TYR:CE2	3:D:390:CYS:HA	2.54	0.43
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.84	0.43
1:C:38:ASP:HB3	1:C:41:THR:OG1	2.19	0.43
2:B:323:GLN:HA	2:B:324:PRO:HA	1.76	0.43
3:D:203:GLN:HA	3:D:204:PRO:HD3	1.83	0.43
1:A:200:ARG:NH2	6:A:2088:HOH:O	2.51	0.43
4:C:1295:T7Z:N32	4:C:1295:T7Z:H061	2.32	0.43
1:C:127:ASP:HB2	1:C:148:LEU:HD12	2.00	0.43
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:CG	1:A:74:ASN:N	2.79	0.43
2:B:177:ASP:OD1	2:B:177:ASP:O	2.37	0.43
3:D:207:THR:OG1	3:D:210:MET:HG3	2.18	0.43
1:A:101:LEU:HB3	1:A:102:PRO:HD3	2.00	0.42
1:A:195:GLU:O	1:A:199:ARG:N	2.50	0.42
1:C:165:THR:O	1:C:166:LEU:C	2.58	0.42
1:C:181:SER:OG	1:C:182:THR:N	2.50	0.42
3:D:311:VAL:O	3:D:315:LEU:HG	2.18	0.42
2:B:388:LYS:O	2:B:392:MET:HG2	2.19	0.42
2:B:202:LYS:O	2:B:204:PRO:HD3	2.18	0.42
2:B:214:LEU:HD22	2:B:253:LEU:HG	2.01	0.42
2:B:211:ARG:HD3	2:B:344:ALA:HB2	2.02	0.42
1:C:127:ASP:CG	1:C:148:LEU:HD12	2.40	0.42
3:D:414:LYS:HA	3:D:420:GLY:HA2	2.02	0.42
1:C:231:THR:HA	1:C:236:TYR:CG	2.53	0.42
1:C:88:LYS:HA	1:C:88:LYS:HD2	1.86	0.42
1:A:53:SER:HB3	2:B:304:PHE:O	2.20	0.42
3:D:376:LEU:HD23	3:D:376:LEU:HA	1.86	0.42
1:C:61:PRO:O	1:C:142:LYS:HE2	2.20	0.42
1:C:52:ILE:HD11	1:C:78:LEU:HD21	2.02	0.42
1:A:230:VAL:O	1:A:233:MET:HG3	2.20	0.42
3:D:372:TRP:CZ3	3:D:376:LEU:HD13	2.55	0.42
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.54	0.41
1:C:55:LEU:HA	1:C:55:LEU:HD12	1.87	0.41
3:D:262:LEU:HD13	3:D:278:PHE:CD2	2.56	0.41
1:A:193:PHE:O	1:A:197:VAL:HG23	2.21	0.41
1:A:60:HIS:HD2	1:A:117:PHE:CD1	2.38	0.41
1:C:105:LYS:HB2	1:C:105:LYS:HE3	1.76	0.41
3:D:373:PRO:O	3:D:377:ILE:HG13	2.20	0.41
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.02	0.41
3:D:223:GLU:OE1	3:D:412:LYS:HE3	2.20	0.41
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.35	0.41
3:D:415:ASN:OD1	3:D:416:SER:N	2.54	0.41
1:A:11:GLY:HA3	4:A:1297:T7Z:C20	2.51	0.41
1:A:83:LEU:O	4:A:1297:T7Z:N11	2.54	0.41
1:C:70:ILE:HB	1:C:77:TYR:HB2	2.02	0.41
1:A:178:LYS:HD3	1:A:179:TYR:CE2	2.55	0.41
2:B:176:PRO:N	2:B:179[B]:HIS:CD2	2.89	0.41
2:B:345:ASP:HA	2:B:346:PRO:HA	1.65	0.41
1:C:108:LEU:HD22	1:C:193:PHE:CD1	2.56	0.41
2:B:344:ALA:O	2:B:348:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:PRO:O	2:B:349:LYS:HG2	2.20	0.41
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.80	0.40
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.57	0.40
3:D:239:ILE:HD11	3:D:257:GLY:HA2	2.03	0.40
1:C:150:ARG:NH2	3:D:268:GLU:O	2.54	0.40
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.56	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	291/301 (97%)	278 (96%)	12 (4%)	1 (0%)	41 49
1	C	292/301 (97%)	269 (92%)	20 (7%)	3 (1%)	15 16
2	B	256/262 (98%)	253 (99%)	3 (1%)	0	100 100
3	D	230/262 (88%)	219 (95%)	10 (4%)	1 (0%)	34 41
All	All	1069/1126 (95%)	1019 (95%)	45 (4%)	5 (0%)	29 34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	LEU
1	C	164	VAL
1	A	164	VAL
1	C	256	ASP
3	D	420	GLY

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	259/264 (98%)	251 (97%)	8 (3%)	40	52
1	C	259/264 (98%)	254 (98%)	5 (2%)	57	69
2	B	232/236 (98%)	230 (99%)	2 (1%)	78	86
3	D	212/236 (90%)	209 (99%)	3 (1%)	67	77
All	All	962/1000 (96%)	944 (98%)	18 (2%)	57	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	73	GLU
1	A	122	ARG
1	A	150	ARG
1	A	206	ASP
1	A	248	PHE
1	A	295	HIS
1	A	296	LEU
2	B	209	SER
2	B	374	GLU
1	C	36	ARG
1	C	122	ARG
1	C	199	ARG
1	C	218	THR
1	C	248	PHE
3	D	338	GLU
3	D	398	TYR
3	D	424	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	317	GLN

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Mol	Chain	Res	Type
3	D	419	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	C	160	1	8,10,11	0.79	0	10,14,16	1.28	0
1	TPO	A	160	1	8,10,11	0.82	0	10,14,16	1.35	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	-

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	A	160	TPO	CG2-CB-CA	-2.39	108.46	113.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
5	SGM	B	1433	-	5,5,5	0.44	0	5,5,5	0.41	0
5	SGM	D	1429	-	5,5,5	0.36	0	5,5,5	0.85	0
4	T7Z	A	1297	-	30,36,36	3.49	9 (30%)	37,52,52	3.33	14 (37%)
4	T7Z	C	1295	-	30,36,36	3.51	9 (30%)	37,52,52	2.95	16 (43%)

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
5	SGM	B	1433	-	-	0/4/4/4	-
5	SGM	D	1429	-	-	0/4/4/4	-
4	T7Z	A	1297	-	-	4/17/32/32	0/4/4/4
4	T7Z	C	1295	-	-	6/17/32/32	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1297	T7Z	C17-N16	-11.71	1.35	1.47
4	C	1295	T7Z	C17-N16	-11.67	1.35	1.47
4	C	1295	T7Z	C21-N16	-11.66	1.35	1.47
4	A	1297	T7Z	C21-N16	-11.48	1.35	1.47
4	C	1295	T7Z	C10-N11	4.60	1.45	1.36
4	C	1295	T7Z	C03-N02	4.31	1.47	1.33
4	A	1297	T7Z	C03-N02	4.26	1.47	1.33
4	A	1297	T7Z	C10-N11	3.97	1.44	1.36
4	A	1297	T7Z	C30-C31	3.71	1.50	1.44
4	C	1295	T7Z	C30-C31	3.33	1.49	1.44
4	A	1297	T7Z	C14-S15	2.94	1.82	1.78
4	A	1297	T7Z	C12-N11	2.86	1.47	1.40
4	C	1295	T7Z	C12-N11	2.85	1.47	1.40
4	C	1295	T7Z	C14-S15	2.73	1.81	1.78
4	A	1297	T7Z	C13-C14	2.62	1.43	1.39
4	A	1297	T7Z	C08-C07	2.41	1.54	1.49
4	C	1295	T7Z	C08-C07	2.34	1.54	1.49
4	C	1295	T7Z	C13-C14	2.30	1.42	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1297	T7Z	C21-N16-C17	11.25	124.61	112.17
4	C	1295	T7Z	C21-N16-C17	8.46	121.53	112.17
4	A	1297	T7Z	C20-C21-N16	7.94	112.86	108.18
4	C	1295	T7Z	N28-C10-N09	-6.95	119.96	126.55
4	A	1297	T7Z	O23-S15-O22	-6.50	108.99	119.52
4	C	1295	T7Z	O23-S15-O22	-6.22	109.44	119.52
4	A	1297	T7Z	O22-S15-N16	6.05	112.20	106.69
4	A	1297	T7Z	N28-C10-N09	-5.61	121.24	126.55
4	C	1295	T7Z	C18-C17-N16	4.71	110.95	108.18
4	A	1297	T7Z	C18-C17-N16	4.53	110.84	108.18
4	A	1297	T7Z	C17-N16-S15	-4.30	109.24	117.05
4	C	1295	T7Z	C17-N16-S15	-4.10	109.59	117.05
4	C	1295	T7Z	C26-C24-C14	3.98	120.68	116.27
4	C	1295	T7Z	C29-N28-C10	3.79	121.60	115.88
4	C	1295	T7Z	C25-C24-C14	-3.71	120.53	124.16
4	A	1297	T7Z	C26-C24-C14	3.49	120.14	116.27
4	A	1297	T7Z	C29-N28-C10	3.35	120.93	115.88
4	C	1295	T7Z	O23-S15-N16	3.25	109.66	106.69
4	C	1295	T7Z	C20-C21-N16	3.00	109.95	108.18
4	C	1295	T7Z	O22-S15-N16	2.93	109.36	106.69
4	C	1295	T7Z	C01-N02-C03	2.89	120.41	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1295	T7Z	C21-N16-S15	2.69	121.94	117.05
4	C	1295	T7Z	C30-C29-N28	-2.66	119.44	123.42
4	A	1297	T7Z	C30-C29-N28	-2.63	119.48	123.42
4	C	1295	T7Z	C24-C14-S15	-2.28	119.96	122.05
4	A	1297	T7Z	C07-C08-N09	2.20	117.73	115.03
4	A	1297	T7Z	C01-N02-C03	2.08	119.64	117.66
4	C	1295	T7Z	C13-C14-S15	2.07	120.16	117.57
4	A	1297	T7Z	O23-S15-C14	2.07	111.36	107.36
4	A	1297	T7Z	C24-C14-S15	-2.04	120.18	122.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1295	T7Z	C17-N16-S15-C14
4	C	1295	T7Z	C17-N16-S15-O22
4	C	1295	T7Z	C17-N16-S15-O23
4	A	1297	T7Z	C17-N16-S15-O23
4	A	1297	T7Z	N09-C10-N11-C12
4	A	1297	T7Z	N28-C10-N11-C12
4	A	1297	T7Z	C17-N16-S15-C14
4	C	1295	T7Z	N09-C10-N11-C12
4	C	1295	T7Z	N28-C10-N11-C12
4	C	1295	T7Z	C21-N16-S15-O22

There are no ring outliers.

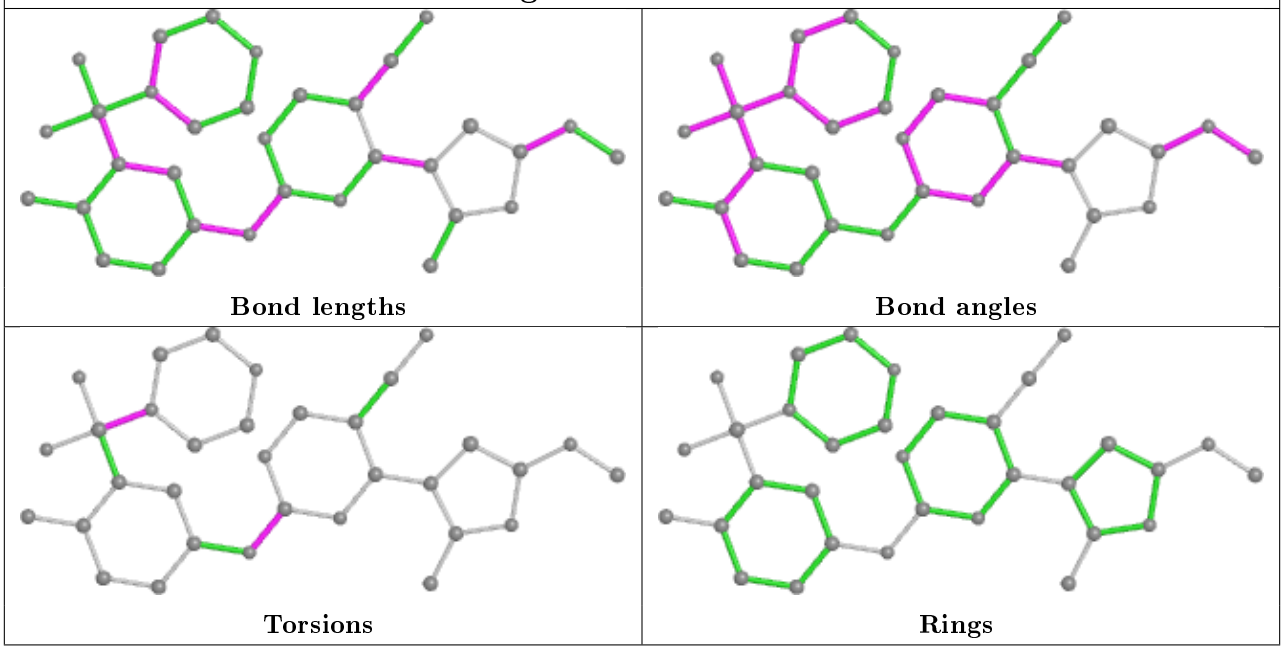
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1433	SGM	2	0
5	D	1429	SGM	2	0
4	A	1297	T7Z	8	0
4	C	1295	T7Z	4	0

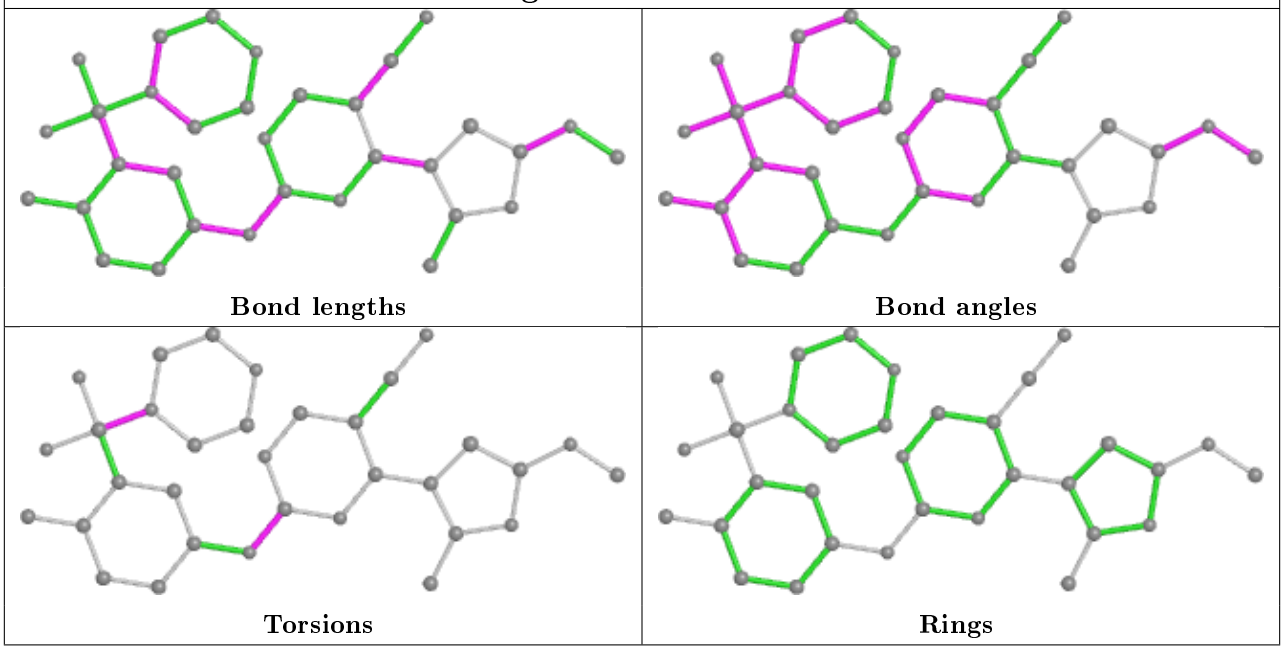
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 T7Z A 1297



Ligand T7Z C 1295



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	295/301 (98%)	0.04	3 (1%) 82 83	19, 31, 83, 116	0
1	C	294/301 (97%)	0.77	45 (15%) 2 1	30, 68, 103, 118	0
2	B	257/262 (98%)	-0.02	3 (1%) 79 77	18, 33, 58, 93	0
3	D	236/262 (90%)	0.88	45 (19%) 1 0	27, 64, 99, 115	0
All	All	1082/1126 (96%)	0.41	96 (8%) 9 6	18, 47, 96, 118	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	418	TYR	6.1
1	C	215	ILE	5.9
3	D	372	TRP	5.7
3	D	423	LEU	5.2
3	D	333	ALA	5.0
3	D	332	LEU	4.9
1	C	227	TRP	4.8
1	A	-2	PRO	4.8
3	D	421	VAL	4.7
1	C	236	TYR	4.4
3	D	359	ALA	4.4
1	C	209	ILE	4.3
1	C	226	VAL	4.2
1	C	234	PRO	4.2
3	D	319	PHE	4.2
3	D	413	TYR	4.1
3	D	416	SER	4.1
3	D	336	LEU	4.1
1	C	101	LEU	3.8
1	C	213	PHE	3.7
1	C	173	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
3	D	361	HIS	3.7
1	C	175	LEU	3.7
1	C	170	ALA	3.7
1	C	252	VAL	3.6
3	D	411	GLU	3.6
1	C	216	PHE	3.5
1	C	240	PHE	3.5
1	C	243	TRP	3.4
3	D	419	HIS	3.3
3	D	399	LEU	3.3
1	C	251	VAL	3.3
1	C	239	SER	3.2
1	C	179	TYR	3.2
1	C	282	ALA	3.2
1	C	231	THR	3.1
3	D	318	TYR	3.1
3	D	377	ILE	3.1
3	D	176	PRO	3.1
3	D	335	PHE	3.0
1	C	233	MET	3.0
3	D	395	HIS	2.9
3	D	360	PHE	2.9
1	C	235	ASP	2.8
1	C	287	GLN	2.8
3	D	417	LYS	2.8
3	D	384	LEU	2.7
1	C	290	THR	2.7
3	D	179	HIS	2.7
1	C	247	ASP	2.7
3	D	374	GLU	2.7
3	D	331	LEU	2.7
1	C	293	VAL	2.6
3	D	422	SER	2.6
3	D	426	PRO	2.6
1	C	286	PHE	2.6
3	D	224	GLU	2.6
1	C	250	LYS	2.6
3	D	397	THR	2.5
3	D	420	GLY	2.5
2	B	284	ASP	2.5
1	A	14	THR	2.5
1	C	284	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	212	LEU	2.5
3	D	428	GLU	2.5
3	D	312	ASN	2.5
1	C	102	PRO	2.4
3	D	414	LYS	2.4
3	D	415	ASN	2.4
1	C	268	HIS	2.4
1	C	273	LYS	2.4
1	C	255	LEU	2.4
3	D	404	HIS	2.3
1	C	277	ALA	2.3
1	C	232	SER	2.3
3	D	376	LEU	2.3
3	D	280	TYR	2.3
2	B	280	TYR	2.3
3	D	391	LEU	2.3
3	D	357	GLY	2.2
1	C	238	PRO	2.2
1	C	256	ASP	2.2
3	D	177	ASP	2.2
1	A	15	TYR	2.2
3	D	409	ILE	2.2
2	B	283	ASP	2.2
1	C	245	ARG	2.2
1	C	285	PHE	2.1
1	C	15	TYR	2.1
1	C	187	TRP	2.1
3	D	223	GLU	2.1
1	C	166	LEU	2.1
1	C	161	HIS	2.1
1	C	237	LYS	2.1
3	D	392	MET	2.1
3	D	381	GLY	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^{th} 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	0.93	0.16	50,58,69,71	0
1	TPO	A	160	11/12	0.98	0.13	20,30,33,33	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

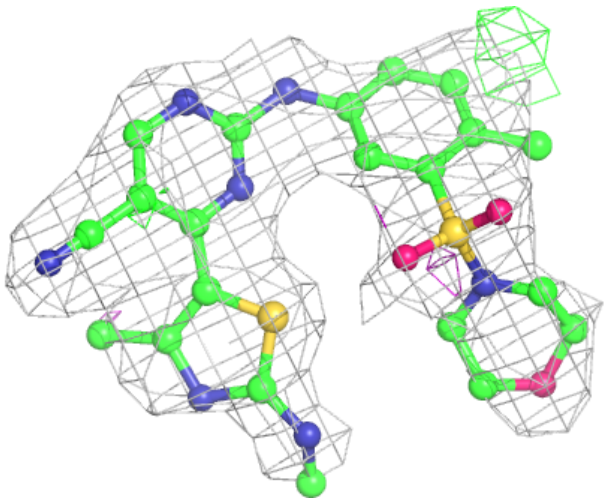
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

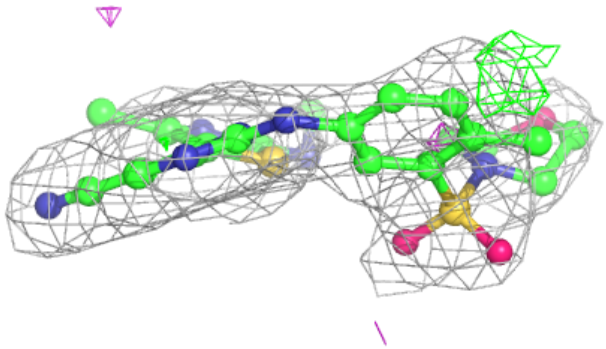
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SGM	D	1429	6/6	0.84	0.30	69,70,73,85	0
4	T7Z	C	1295	33/33	0.89	0.19	37,65,103,105	0
5	SGM	B	1433	6/6	0.92	0.23	50,58,59,61	0
4	T7Z	A	1297	33/33	0.94	0.17	33,43,105,106	0

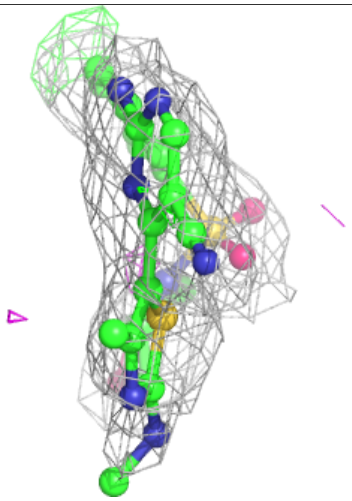
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T7Z C 1295:

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

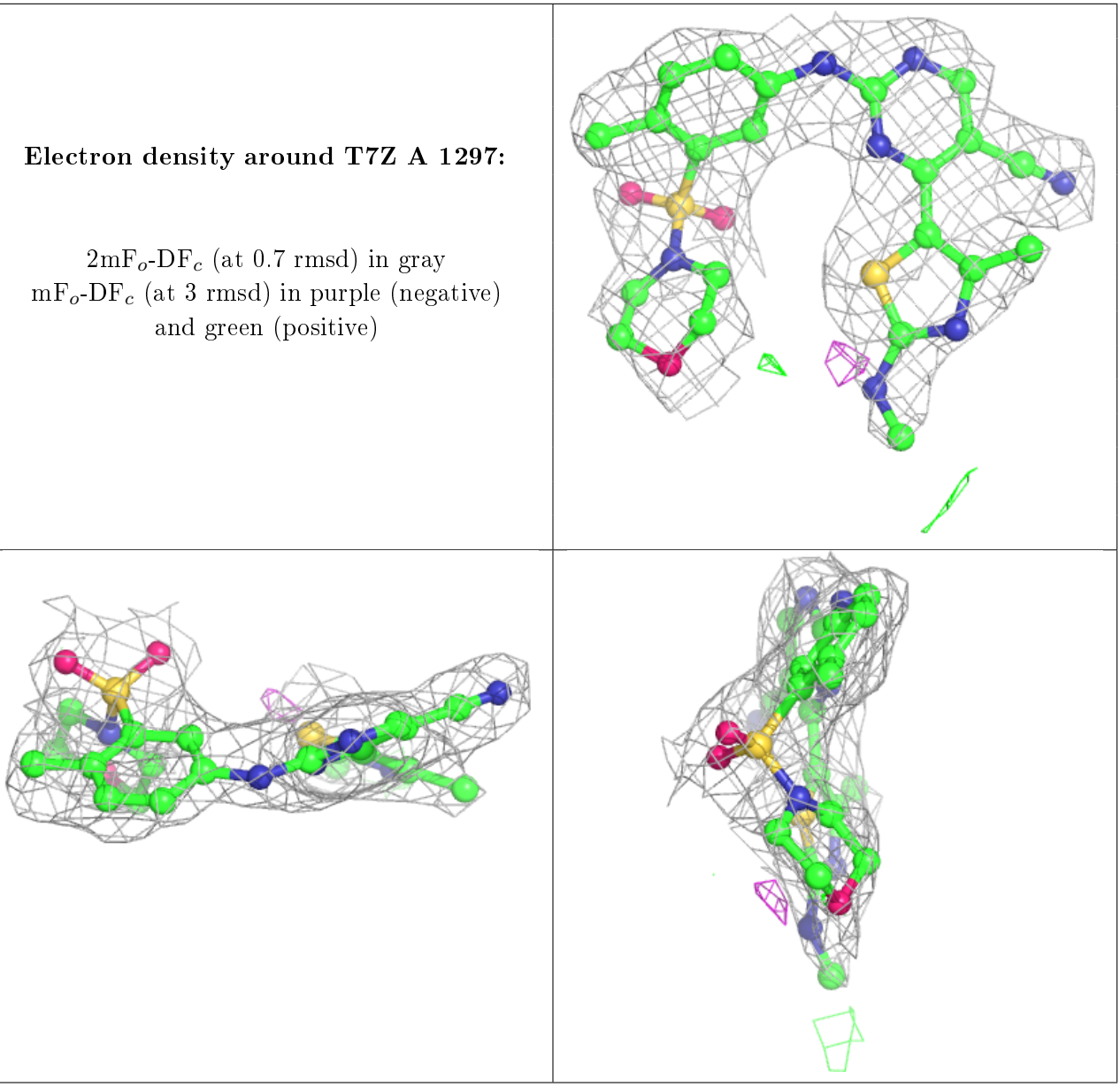






Electron density around T7Z A 1297:

$2mF_o$-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

There are no such residues in this entry.