



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:05 AM UTC

PDB ID : 1P73 / pdb_00001p73
Title : Crystal structure of EHV4-TK complexed with TP4A
Authors : Gardberg, A.; Shuvalova, L.; Monnerjahn, C.; Konrad, M.; Lavie, A.
Deposited on : 2003-04-30
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

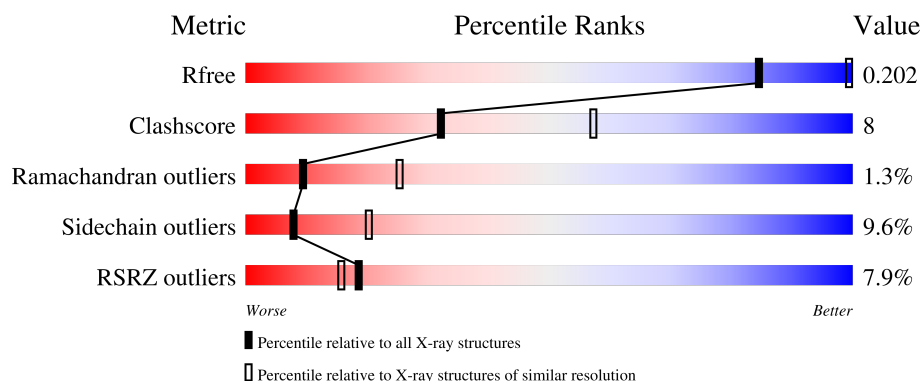
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	334	7% 75% 18% • •
1	B	334	11% 81% 13% • •
1	C	334	5% 77% 18% 5%
1	D	334	7% 75% 20% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10196 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 Thymidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	1	0
			2429	1545	430	436	18			
1	B	329	Total	C	N	O	S	0	0	0
			2506	1587	439	463	17			
1	C	317	Total	C	N	O	S	0	1	0
			2419	1541	424	436	18			
1	D	326	Total	C	N	O	S	0	0	0
			2436	1551	427	441	17			

There are 16 discrepancies between the modelled and reference sequences:

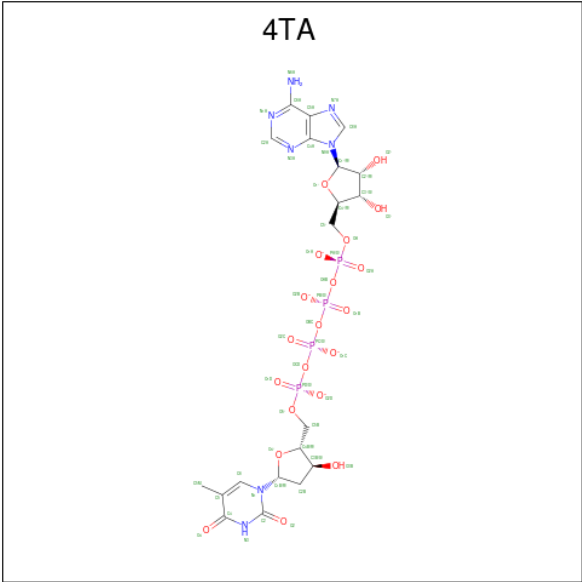
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	cloning artifact	UNP P24425
A	20	SER	-	cloning artifact	UNP P24425
A	21	HIS	-	cloning artifact	UNP P24425
A	22	MET	-	cloning artifact	UNP P24425
B	19	GLY	-	cloning artifact	UNP P24425
B	20	SER	-	cloning artifact	UNP P24425
B	21	HIS	-	cloning artifact	UNP P24425
B	22	MET	-	cloning artifact	UNP P24425
C	19	GLY	-	cloning artifact	UNP P24425
C	20	SER	-	cloning artifact	UNP P24425
C	21	HIS	-	cloning artifact	UNP P24425
C	22	MET	-	cloning artifact	UNP P24425
D	19	GLY	-	cloning artifact	UNP P24425
D	20	SER	-	cloning artifact	UNP P24425
D	21	HIS	-	cloning artifact	UNP P24425
D	22	MET	-	cloning artifact	UNP P24425

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is P1-(5'-ADENOSYL)P4-(5'-(2'-DEOXY-THYMIDYL))TETRAPHOSPHATE (CCD ID: 4TA) (formula: C₂₀H₂₅N₇O₂₀P₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			51	20	7	20	4		
3	B	1	Total	C	N	O	P	0	0
			51	20	7	20	4		
3	C	1	Total	C	N	O	P	0	0
			51	20	7	20	4		
3	D	1	Total	C	N	O	P	0	0
			51	20	7	20	4		

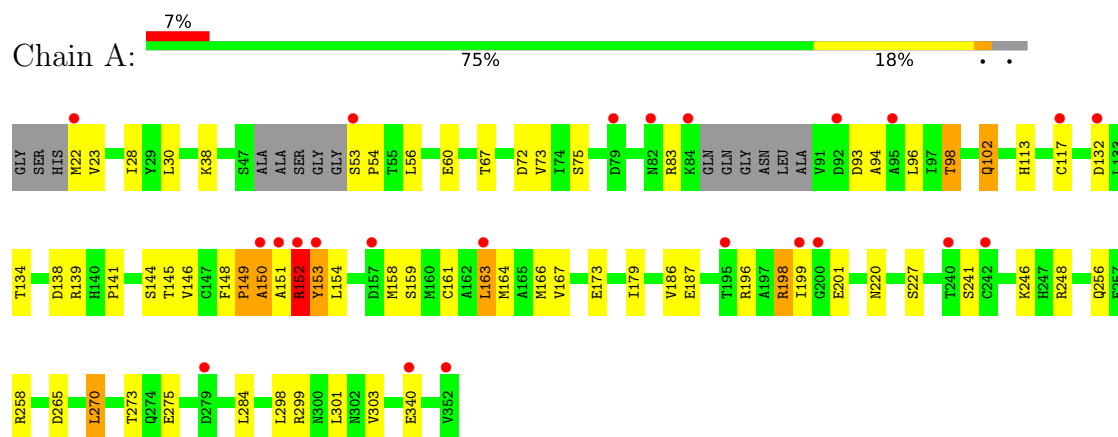
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	38	Total	O	0	0
			38	38		
4	C	30	Total	O	0	0
			30	30		
4	D	45	Total	O	0	0
			45	45		

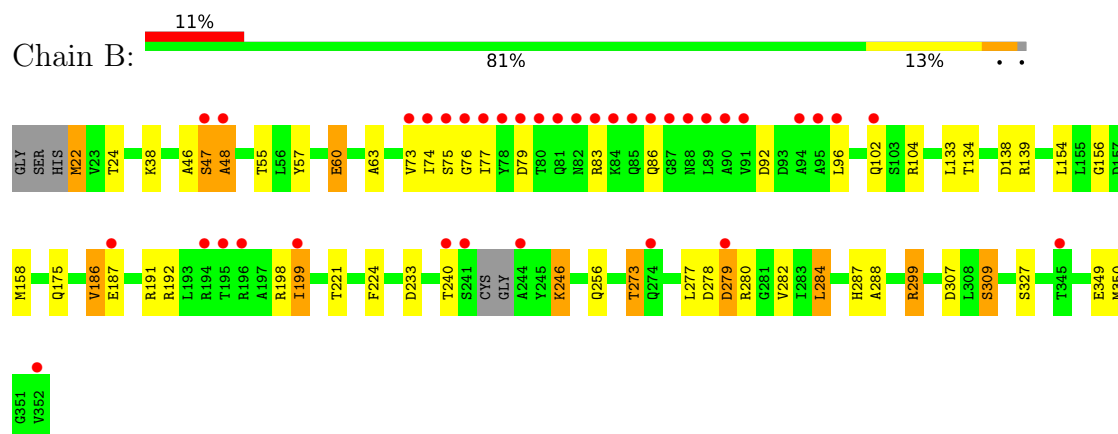
3 Residue-property plots [i](#)

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.

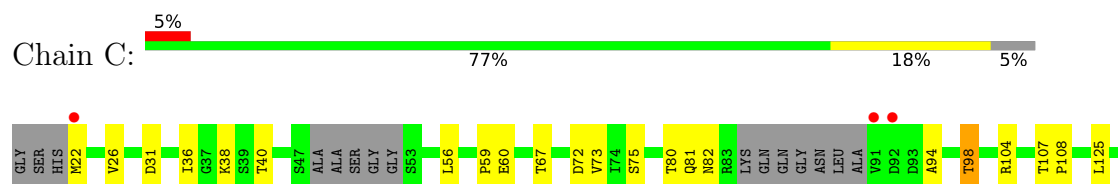
• Molecule 1: Thymidine kinase

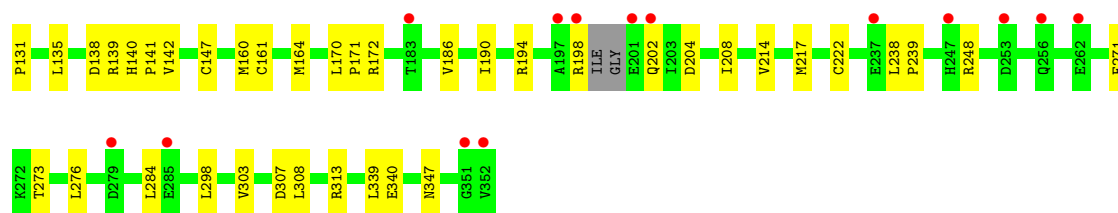


• Molecule 1: Thymidine kinase

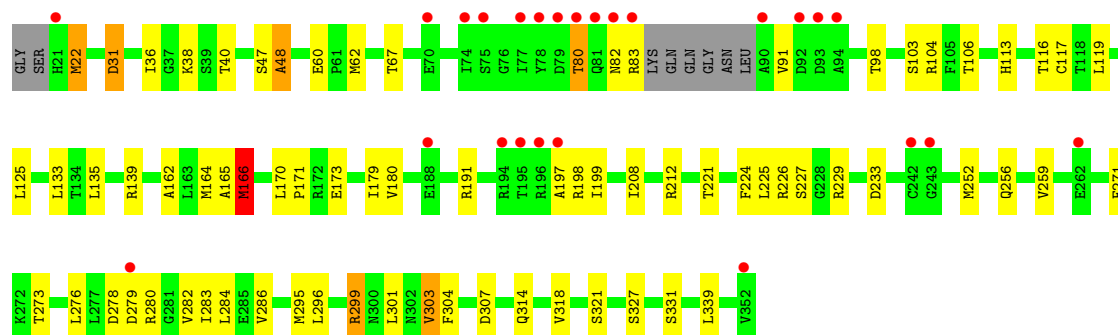
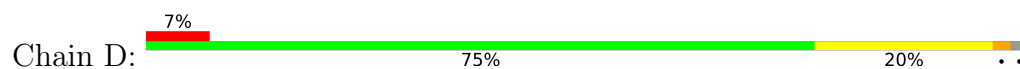


• Molecule 1: Thymidine kinase





● Molecule 1: Thymidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.35Å 118.29Å 122.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.70 29.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.68-2.70) 98.4 (29.68-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.213 , 0.276 0.219 , 0.202	Depositor DCC
R_{free} test set	4458 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10196	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 4TA

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	0.64	1/2482 (0.0%)	0.95	1/3377 (0.0%)
1	B	0.62	0/2557	0.95	2/3480 (0.1%)
1	C	0.60	1/2470 (0.0%)	0.92	1/3361 (0.0%)
1	D	0.61	1/2487 (0.0%)	0.95	0/3391
All	All	0.62	3/9996 (0.0%)	0.95	4/13609 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	MET	SD-CE	5.64	1.93	1.79
1	C	164	MET	SD-CE	5.17	1.92	1.79
1	A	166	MET	SD-CE	5.16	1.92	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ARG	N-CA-C	-6.15	106.13	113.21
1	B	186	VAL	CB-CA-C	-5.37	105.01	112.04
1	C	147	CYS	N-CA-C	5.32	116.77	110.97
1	B	288	ALA	N-CA-C	-5.14	105.75	111.36

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	2429	0	2376	66	0
1	B	2506	0	2441	31	0
1	C	2419	0	2368	28	0
1	D	2436	0	2352	35	0
2	A	20	0	0	0	0
2	B	20	0	0	1	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
3	A	51	0	25	1	0
3	B	51	0	25	1	0
3	C	51	0	25	1	0
3	D	51	0	25	1	0
4	A	34	0	0	4	0
4	B	38	0	0	5	0
4	C	30	0	0	1	0
4	D	45	0	0	4	0
All	All	10196	0	9637	158	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 8.

All (158) 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:A:151:ALA:N	1:A:163:LEU:HG	1.30	1.41
1:A:151:ALA:CA	1:A:163:LEU:HG	1.55	1.36
1:D:117:CYS:HB2	4:D:834:HOH:O	1.41	1.16
1:A:150:ALA:HB1	1:A:167:VAL:HG22	1.32	1.06
1:A:151:ALA:H	1:A:163:LEU:CG	1.68	1.05
1:A:151:ALA:HA	1:A:163:LEU:HG	1.30	1.05
1:A:151:ALA:N	1:A:163:LEU:CG	2.19	1.04
1:A:151:ALA:HA	1:A:163:LEU:CG	1.88	1.03
1:A:146:VAL:HA	1:A:150:ALA:CB	1.91	1.00
1:A:153:TYR:HB3	1:A:163:LEU:CD2	1.90	1.00
1:A:151:ALA:CA	1:A:163:LEU:CG	2.43	0.95
1:A:151:ALA:HA	1:A:163:LEU:CD2	1.99	0.92
1:A:146:VAL:HA	1:A:150:ALA:HB3	1.49	0.92
1:A:94:ALA:O	1:A:98:THR:HG22	1.70	0.92
1:A:150:ALA:CB	1:A:167:VAL:HG22	2.01	0.89
1:A:150:ALA:HB1	1:A:167:VAL:CG2	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ALA:H	1:A:163:LEU:HG	1.04	0.84
1:A:153:TYR:HB3	1:A:163:LEU:HD23	1.61	0.80
1:B:102:GLN:NE2	4:B:828:HOH:O	2.14	0.79
1:B:47:SER:O	1:B:48:ALA:CB	2.31	0.78
1:B:299:ARG:HG3	1:B:299:ARG:HH11	1.48	0.78
1:D:212:ARG:HD3	1:D:252:MET:HE1	1.64	0.78
1:C:94:ALA:O	1:C:98:THR:HG22	1.85	0.77
1:A:198:ARG:H	1:A:201:GLU:HG3	1.52	0.74
1:A:146:VAL:HA	1:A:150:ALA:HB2	1.67	0.74
1:A:153:TYR:HB3	1:A:163:LEU:HD21	1.70	0.73
1:C:73:VAL:HG11	1:C:104:ARG:HB3	1.73	0.70
1:A:152:ARG:C	1:A:154:LEU:H	2.00	0.70
1:B:76:GLY:HA2	4:B:826:HOH:O	1.92	0.70
1:C:170:LEU:HD12	1:C:171:PRO:HD2	1.74	0.69
1:B:299:ARG:HH11	1:B:299:ARG:CG	2.05	0.69
1:A:149:PRO:O	1:A:152:ARG:N	2.28	0.67
1:D:103:SER:HA	1:D:166:MET:HE1	1.76	0.67
1:A:146:VAL:CA	1:A:150:ALA:HB3	2.24	0.66
1:A:151:ALA:CB	1:A:270:LEU:HD11	2.24	0.66
1:D:47:SER:O	1:D:48:ALA:CB	2.44	0.66
1:A:159:SER:O	1:A:163:LEU:HD22	1.96	0.65
1:A:152:ARG:HG2	1:A:152:ARG:O	1.97	0.65
1:A:179:ILE:HG23	1:A:303:VAL:HG23	1.79	0.64
1:D:135:LEU:HD11	1:D:339:LEU:HD13	1.79	0.64
1:A:153:TYR:HA	1:A:158:MET:O	1.99	0.63
1:B:307:ASP:OD2	1:B:309:SER:HB2	1.99	0.63
1:B:47:SER:O	1:B:48:ALA:HB2	1.99	0.63
1:B:102:GLN:HG2	1:B:158:MET:HE1	1.81	0.62
1:A:145:THR:O	1:A:150:ALA:HB2	2.00	0.62
1:A:150:ALA:CB	1:A:167:VAL:CG2	2.71	0.61
1:B:278:ASP:HB2	1:B:282:VAL:H	1.66	0.61
1:B:299:ARG:HG3	1:B:299:ARG:NH1	2.12	0.61
1:A:164:MET:HE2	4:A:830:HOH:O	2.00	0.60
1:B:154:LEU:HA	1:B:246:LYS:HE3	1.83	0.60
1:A:153:TYR:N	1:A:163:LEU:HD21	2.18	0.59
1:A:161:CYS:SG	1:B:104:ARG:HD3	2.43	0.59
1:A:151:ALA:CB	1:A:270:LEU:CD1	2.82	0.58
1:C:60:GLU:OE1	3:C:803:4TA:O1D	2.22	0.58
1:A:148:PHE:O	1:A:152:ARG:HB2	2.03	0.58
1:D:104:ARG:HD3	4:D:836:HOH:O	2.03	0.58
1:A:146:VAL:O	1:A:150:ALA:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:GLN:O	1:D:318:VAL:HG23	2.05	0.57
1:C:72:ASP:HB3	1:C:75:SER:HB2	1.87	0.57
1:C:161:CYS:SG	1:D:104:ARG:NH1	2.77	0.56
1:A:164:MET:CE	4:A:830:HOH:O	2.51	0.56
1:A:151:ALA:HB3	1:A:270:LEU:HD11	1.86	0.55
1:A:151:ALA:C	1:A:153:TYR:H	2.13	0.55
1:D:173:GLU:HG2	1:D:301:LEU:HD21	1.88	0.55
1:D:47:SER:O	1:D:48:ALA:HB2	2.06	0.55
1:A:149:PRO:HA	1:A:152:ARG:HB3	1.87	0.54
1:A:153:TYR:H	1:A:163:LEU:HD21	1.70	0.54
1:D:113:HIS:CE1	1:D:117:CYS:SG	3.00	0.54
1:A:151:ALA:H	1:A:163:LEU:CB	2.19	0.54
1:A:256:GLN:HE21	1:A:258:ARG:CZ	2.21	0.54
1:A:275:GLU:HB2	4:A:833:HOH:O	2.08	0.54
1:B:79:ASP:O	1:B:83:ARG:HG3	2.08	0.54
1:C:80:THR:C	1:C:82:ASN:H	2.15	0.54
1:B:76:GLY:CA	4:B:826:HOH:O	2.51	0.53
1:B:46:ALA:HB2	1:B:57:TYR:HB2	1.91	0.53
1:A:23:VAL:HG13	1:A:132:ASP:HB2	1.91	0.52
1:D:173:GLU:HG2	1:D:301:LEU:CD2	2.40	0.52
1:A:152:ARG:C	1:A:154:LEU:N	2.62	0.52
1:D:278:ASP:HB3	1:D:280:ARG:H	1.75	0.52
1:A:152:ARG:O	1:A:152:ARG:CG	2.57	0.51
1:B:156:GLY:HA2	4:B:821:HOH:O	2.10	0.51
1:A:144:SER:O	1:A:149:PRO:HG3	2.10	0.51
1:A:220:ASN:HD22	1:A:265:ASP:HB3	1.76	0.51
1:A:56:LEU:HD11	1:A:340:GLU:HG3	1.94	0.50
1:A:151:ALA:N	1:A:163:LEU:CD1	2.74	0.50
1:D:278:ASP:HB2	1:D:282:VAL:H	1.77	0.49
1:B:198:ARG:O	1:B:199:ILE:C	2.55	0.49
1:D:299:ARG:HD2	4:D:840:HOH:O	2.12	0.49
1:A:151:ALA:HA	1:A:163:LEU:HD23	1.91	0.49
1:B:60:GLU:OE1	3:B:802:4TA:O1D	2.29	0.49
1:A:138:ASP:O	1:A:139:ARG:HB2	2.14	0.48
1:C:186:VAL:HG22	1:C:190:ILE:HD11	1.96	0.47
1:D:80:THR:C	1:D:82:ASN:H	2.21	0.47
1:C:60:GLU:HG3	1:C:138:ASP:CG	2.40	0.47
1:B:273:THR:O	1:B:277:LEU:HG	2.15	0.47
1:C:94:ALA:O	1:C:98:THR:CG2	2.60	0.47
1:C:38:LYS:HB3	1:C:38:LYS:HE3	1.72	0.46
1:C:135:LEU:HD11	1:C:339:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:C	1:A:270:LEU:HD12	2.40	0.46
1:B:138:ASP:O	1:B:139:ARG:HB2	2.16	0.46
1:B:175:GLN:HG2	2:B:607:SO4:O3	2.16	0.46
1:B:284:LEU:HB2	1:B:287:HIS:CD2	2.50	0.46
1:A:102:GLN:HG2	1:A:149:PRO:HB3	1.97	0.46
1:C:59:PRO:HD3	1:C:347:ASN:OD1	2.16	0.45
1:C:36:ILE:HG22	1:C:308:LEU:HD12	1.98	0.45
1:D:225:LEU:HD22	1:D:295:MET:HG3	1.98	0.45
1:A:151:ALA:HB1	1:A:270:LEU:HD13	1.98	0.45
1:B:47:SER:O	1:B:48:ALA:HB3	2.12	0.45
1:D:197:ALA:O	1:D:198:ARG:C	2.60	0.45
1:D:80:THR:HA	1:D:82:ASN:ND2	2.32	0.44
1:C:138:ASP:O	1:C:139:ARG:HB2	2.17	0.44
1:D:22:MET:HA	1:D:331:SER:O	2.17	0.44
1:D:60:GLU:OE1	3:D:804:4TA:O1D	2.35	0.44
1:A:149:PRO:HA	1:A:152:ARG:CB	2.48	0.44
1:D:162:ALA:O	1:D:165:ALA:HB3	2.18	0.44
1:D:162:ALA:O	1:D:166:MET:HG2	2.18	0.44
1:C:73:VAL:HG11	1:C:104:ARG:CB	2.44	0.44
1:D:166:MET:HE2	1:D:166:MET:HB3	1.89	0.44
1:B:278:ASP:HB3	1:B:280:ARG:H	1.83	0.44
1:D:103:SER:O	1:D:106:THR:HB	2.17	0.44
1:B:55:THR:HA	1:B:134:THR:O	2.18	0.43
1:B:279:ASP:OD1	1:B:279:ASP:N	2.51	0.43
1:D:82:ASN:OD1	1:D:83:ARG:N	2.52	0.43
1:B:63:ALA:HB3	1:B:350:MET:HA	1.99	0.43
1:D:80:THR:CB	4:D:829:HOH:O	2.65	0.43
1:A:146:VAL:C	1:A:150:ALA:HB3	2.44	0.43
1:A:152:ARG:H	1:A:163:LEU:HD11	1.83	0.43
1:C:271:PHE:O	1:C:276:LEU:HD12	2.17	0.43
1:D:179:ILE:HG23	1:D:303:VAL:HG23	2.00	0.43
1:B:221:THR:O	1:B:224:PHE:HB3	2.18	0.43
1:B:349:GLU:O	1:B:350:MET:HE2	2.18	0.43
1:C:82:ASN:OD1	1:C:82:ASN:C	2.62	0.43
1:C:107:THR:HB	1:C:108:PRO:HD3	2.00	0.42
1:C:140:HIS:HB3	1:C:142:VAL:HG12	2.01	0.42
1:B:92:ASP:O	1:B:96:LEU:HG	2.20	0.42
4:C:831:HOH:O	1:D:164:MET:HE3	2.19	0.42
1:D:180:VAL:HG22	1:D:304:PHE:HB2	2.00	0.42
1:A:173:GLU:HG2	1:A:301:LEU:HD23	2.02	0.42
1:C:140:HIS:CD2	1:C:141:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:HD12	1:D:171:PRO:HD2	2.02	0.42
1:A:72:ASP:HB3	1:A:75:SER:HB2	2.02	0.42
1:C:56:LEU:HD11	1:C:340:GLU:HG3	2.02	0.42
1:A:60:GLU:OE1	3:A:801:4TA:O1D	2.39	0.41
1:C:214:VAL:O	1:C:217:MET:HB2	2.20	0.41
1:A:53:SER:HA	1:A:54:PRO:HD2	1.91	0.41
1:C:26:VAL:HG23	1:C:131:PRO:HB3	2.02	0.41
1:A:151:ALA:C	1:A:153:TYR:N	2.78	0.41
1:D:116:THR:HA	1:D:119:LEU:HD12	2.01	0.41
1:D:271:PHE:O	1:D:276:LEU:HD12	2.20	0.41
1:C:140:HIS:CG	1:C:141:PRO:HD2	2.55	0.41
1:C:238:LEU:HA	1:C:239:PRO:HD2	1.93	0.41
1:A:113:HIS:CE1	1:A:117:CYS:SG	3.14	0.41
1:C:80:THR:C	1:C:82:ASN:N	2.79	0.41
1:D:31:ASP:OD1	1:D:139:ARG:NH1	2.53	0.41
1:D:221:THR:O	1:D:224:PHE:HB3	2.21	0.41
1:A:53:SER:CB	4:A:813:HOH:O	2.69	0.41
1:B:22:MET:N	4:B:808:HOH:O	2.54	0.40
1:C:222:CYS:HB2	1:C:303:VAL:HG11	2.04	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	315/334 (94%)	293 (93%)	16 (5%)	6 (2%)	6	17
1	B	325/334 (97%)	307 (94%)	13 (4%)	5 (2%)	8	22
1	C	310/334 (93%)	299 (96%)	10 (3%)	1 (0%)	36	60
1	D	322/334 (96%)	297 (92%)	20 (6%)	5 (2%)	7	20
All	All	1272/1336 (95%)	1196 (94%)	59 (5%)	17 (1%)	9	25

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	B	199	ILE
1	A	150	ALA
1	A	241	SER
1	B	48	ALA
1	B	233	ASP
1	C	81	GLN
1	D	48	ALA
1	D	80	THR
1	D	199	ILE
1	D	233	ASP
1	A	196	ARG
1	A	199	ILE
1	B	47	SER
1	B	77	ILE
1	A	141	PRO
1	D	91	VAL

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	249/279 (89%)	223 (90%)	26 (10%)	7	17
1	B	259/279 (93%)	237 (92%)	22 (8%)	10	25
1	C	250/279 (90%)	231 (92%)	19 (8%)	12	30
1	D	243/279 (87%)	214 (88%)	29 (12%)	5	13
All	All	1001/1116 (90%)	905 (90%)	96 (10%)	8	20

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	28	ILE
1	A	30	LEU

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Mol	Chain	Res	Type
1	A	38	LYS
1	A	67	THR
1	A	73	VAL
1	A	83	ARG
1	A	93	ASP
1	A	96	LEU
1	A	98	THR
1	A	102	GLN
1	A	134	THR
1	A	152	ARG
1	A	153	TYR
1	A	163	LEU
1	A	186	VAL
1	A	187	GLU
1	A	198	ARG
1	A	227	SER
1	A	246	LYS
1	A	248	ARG
1	A	270	LEU
1	A	273	THR
1	A	284	LEU
1	A	298	LEU
1	A	299	ARG
1	B	22	MET
1	B	24	THR
1	B	38	LYS
1	B	60	GLU
1	B	73	VAL
1	B	74	ILE
1	B	75	SER
1	B	86	GLN
1	B	133	LEU
1	B	186	VAL
1	B	187	GLU
1	B	191	ARG
1	B	192	ARG
1	B	240	THR
1	B	246	LYS
1	B	256	GLN
1	B	273	THR
1	B	279	ASP
1	B	284	LEU

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Mol	Chain	Res	Type
1	B	299	ARG
1	B	309	SER
1	B	327	SER
1	C	22	MET
1	C	31	ASP
1	C	40	THR
1	C	67	THR
1	C	98	THR
1	C	125	LEU
1	C	160	MET
1	C	172	ARG
1	C	194	ARG
1	C	198	ARG
1	C	202	GLN
1	C	204	ASP
1	C	208	ILE
1	C	248	ARG
1	C	273	THR
1	C	284	LEU
1	C	298	LEU
1	C	307	ASP
1	C	313	ARG
1	D	22	MET
1	D	31	ASP
1	D	36	ILE
1	D	38	LYS
1	D	40	THR
1	D	62	MET
1	D	67	THR
1	D	98	THR
1	D	125	LEU
1	D	133	LEU
1	D	166	MET
1	D	191	ARG
1	D	208	ILE
1	D	226	ARG
1	D	227	SER
1	D	229	ARG
1	D	256	GLN
1	D	259	VAL
1	D	273	THR
1	D	279	ASP

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Mol	Chain	Res	Type
1	D	283	ILE
1	D	284	LEU
1	D	286	VAL
1	D	296	LEU
1	D	299	ARG
1	D	303	VAL
1	D	307	ASP
1	D	321	SER
1	D	327	SER

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

Mol	Chain	Res	Type
1	A	126	GLN
1	A	202	GLN
1	A	256	GLN
1	A	302	ASN
1	B	82	ASN
1	B	86	GLN
1	B	185	ASN
1	B	202	GLN
1	B	251	GLN
1	B	302	ASN
1	C	126	GLN
1	D	113	HIS
1	D	185	ASN
1	D	302	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

15 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	$\# Z > 2$
2	SO4	A	601	-	4,4,4	0.25	0	6,6,6	0.33	0
2	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.12	0
3	4TA	A	801	-	55,55,55	1.25	8 (14%)	79,86,86	1.86	16 (20%)
2	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.33	0
2	SO4	B	604	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	A	605	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	C	610	-	4,4,4	0.24	0	6,6,6	0.29	0
3	4TA	D	804	-	55,55,55	1.28	8 (14%)	79,86,86	1.81	14 (17%)
2	SO4	B	608	-	4,4,4	0.24	0	6,6,6	0.10	0
3	4TA	C	803	-	55,55,55	1.44	10 (18%)	79,86,86	1.76	14 (17%)
2	SO4	D	611	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	B	607	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	B	606	-	4,4,4	0.23	0	6,6,6	0.17	0
3	4TA	B	802	-	55,55,55	1.41	10 (18%)	79,86,86	1.83	17 (21%)
2	SO4	C	609	-	4,4,4	0.27	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4TA	B	802	-	-	3/38/66/66	0/5/5/5
3	4TA	C	803	-	-	5/38/66/66	0/5/5/5
3	4TA	A	801	-	-	7/38/66/66	0/5/5/5
3	4TA	D	804	-	-	1/38/66/66	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	803	4TA	C8A-N7A	3.83	1.39	1.31
3	B	802	4TA	PC-OBC	3.82	1.63	1.59
3	A	801	4TA	C8A-N7A	3.79	1.39	1.31
3	D	804	4TA	C8A-N7A	3.69	1.38	1.31
3	C	803	4TA	PD-OCD	3.54	1.63	1.59
3	B	802	4TA	C8A-N7A	3.51	1.38	1.31
3	C	803	4TA	C6-C5	3.40	1.40	1.34
3	D	804	4TA	C6-C5	3.36	1.40	1.34
3	B	802	4TA	C2-N1	3.29	1.43	1.38
3	B	802	4TA	C6-C5	3.02	1.39	1.34
3	A	801	4TA	PB-OBC	2.93	1.62	1.59
3	C	803	4TA	PA-OAB	2.92	1.62	1.59
3	A	801	4TA	PC-OBC	2.90	1.62	1.59
3	B	802	4TA	C4-C5	2.75	1.49	1.44
3	C	803	4TA	PC-OBC	2.74	1.62	1.59
3	D	804	4TA	C4-C5	2.74	1.49	1.44
3	B	802	4TA	PD-OCD	2.74	1.62	1.59
3	A	801	4TA	C6-C5	2.66	1.38	1.34
3	C	803	4TA	C2-N1	2.64	1.42	1.38
3	D	804	4TA	C2-N1	2.62	1.42	1.38
3	B	802	4TA	PC-OCD	2.58	1.62	1.59
3	C	803	4TA	PC-OCD	2.51	1.62	1.59
3	C	803	4TA	C4-C5	2.49	1.48	1.44
3	B	802	4TA	PB-OBC	2.44	1.62	1.59
3	C	803	4TA	PB-OAB	2.35	1.62	1.59
3	A	801	4TA	C2-N1	2.16	1.41	1.38
3	D	804	4TA	C4-N3	-2.15	1.34	1.38
3	A	801	4TA	C4-N3	-2.15	1.34	1.38
3	D	804	4TA	PA-OAB	2.10	1.61	1.59
3	A	801	4TA	C4A-N9A	-2.09	1.33	1.37
3	D	804	4TA	C5A-C4A	-2.08	1.35	1.39
3	A	801	4TA	C4-C5	2.06	1.48	1.44
3	D	804	4TA	PD-OCD	2.05	1.61	1.59
3	B	802	4TA	PA-OAB	2.05	1.61	1.59
3	C	803	4TA	C4-N3	-2.03	1.35	1.38
3	B	802	4TA	C4A-N9A	-2.01	1.33	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	804	4TA	N3-C2-N1	5.73	122.35	114.89
3	A	801	4TA	C4-N3-C2	-5.69	119.88	127.34
3	B	802	4TA	N1A-C2A-N3A	-5.50	120.26	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	4TA	C4-N3-C2	-5.48	120.16	127.34
3	D	804	4TA	C4-N3-C2	-5.41	120.25	127.34
3	A	801	4TA	C5-C4-N3	5.33	119.96	115.32
3	A	801	4TA	N1A-C2A-N3A	-5.32	120.53	128.58
3	A	801	4TA	N3-C2-N1	5.05	121.47	114.89
3	C	803	4TA	N1A-C2A-N3A	-5.03	120.97	128.58
3	D	804	4TA	N1A-C2A-N3A	-4.99	121.03	128.58
3	C	803	4TA	C4-N3-C2	-4.90	120.92	127.34
3	C	803	4TA	C5-C4-N3	4.87	119.55	115.32
3	B	802	4TA	C5-C4-N3	4.83	119.52	115.32
3	B	802	4TA	N3-C2-N1	4.75	121.08	114.89
3	D	804	4TA	C5-C4-N3	4.31	119.07	115.32
3	C	803	4TA	C5A-C4A-N9A	4.22	110.41	105.81
3	C	803	4TA	N3-C2-N1	4.21	120.37	114.89
3	A	801	4TA	C5A-C4A-N9A	4.05	110.22	105.81
3	D	804	4TA	C5A-C4A-N9A	4.00	110.17	105.81
3	C	803	4TA	C5-C6-N1	-3.90	119.08	123.31
3	D	804	4TA	C5A-C4A-N3A	-3.80	121.48	126.72
3	C	803	4TA	C5A-C4A-N3A	-3.80	121.48	126.72
3	A	801	4TA	O4-C4-C5	-3.77	120.61	124.92
3	B	802	4TA	O4-C4-C5	-3.52	120.89	124.92
3	A	801	4TA	C5A-C4A-N3A	-3.46	121.96	126.72
3	B	802	4TA	C5A-C4A-N9A	3.42	109.54	105.81
3	A	801	4TA	C5-C6-N1	-3.38	119.64	123.31
3	D	804	4TA	C5-C6-N1	-3.31	119.72	123.31
3	B	802	4TA	C5A-C4A-N3A	-3.29	122.18	126.72
3	C	803	4TA	O4-C4-C5	-3.18	121.28	124.92
3	B	802	4TA	C5-C6-N1	-3.06	119.99	123.31
3	A	801	4TA	C2A-N3A-C4A	3.01	119.17	111.83
3	B	802	4TA	C4A-N9A-C1'	-2.98	119.66	126.63
3	B	802	4TA	C1'-N9A-C8A	2.98	133.70	127.09
3	B	802	4TA	C2A-N3A-C4A	2.95	119.04	111.83
3	A	801	4TA	C1'-N9A-C8A	2.92	133.57	127.09
3	C	803	4TA	C2A-N3A-C4A	2.90	118.92	111.83
3	D	804	4TA	C2A-N3A-C4A	2.83	118.74	111.83
3	C	803	4TA	C1'-N9A-C8A	2.81	133.34	127.09
3	D	804	4TA	C1'-N9A-C8A	2.81	133.33	127.09
3	D	804	4TA	O4-C4-C5	-2.64	121.90	124.92
3	D	804	4TA	C4A-N9A-C1'	-2.57	120.63	126.63
3	A	801	4TA	C4A-N9A-C1'	-2.56	120.65	126.63
3	C	803	4TA	OCD-PD-O1D	-2.52	103.11	110.70
3	B	802	4TA	OAB-PB-O1B	-2.52	103.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	4TA	O1C-PC-OCD	2.49	114.00	107.27
3	B	802	4TA	O4'-C1B-N1	2.46	112.23	107.86
3	A	801	4TA	O2-C2-N1	-2.45	119.60	122.80
3	D	804	4TA	O2-C2-N3	-2.45	116.97	121.49
3	D	804	4TA	O2D-PD-OCD	2.37	113.69	107.27
3	A	801	4TA	C5M-C5-C4	2.36	121.30	118.78
3	C	803	4TA	O2D-PD-OCD	2.35	113.62	107.27
3	B	802	4TA	O1A-PA-OAB	2.33	113.58	107.27
3	A	801	4TA	O2D-PD-O1D	2.23	122.83	112.44
3	C	803	4TA	C4A-N9A-C1'	-2.17	121.55	126.63
3	A	801	4TA	OAB-PB-O1B	-2.10	104.39	110.70
3	C	803	4TA	OBC-PB-O1B	-2.05	104.53	110.70
3	B	802	4TA	N9A-C8A-N7A	-2.05	111.03	113.94
3	B	802	4TA	O2B-PB-O1B	2.05	121.97	112.44
3	B	802	4TA	C5M-C5-C4	2.04	120.96	118.78
3	D	804	4TA	OCD-PD-O1D	-2.04	104.58	110.70

There are no chirality outliers.

All (16) torsion outliers are listed below:

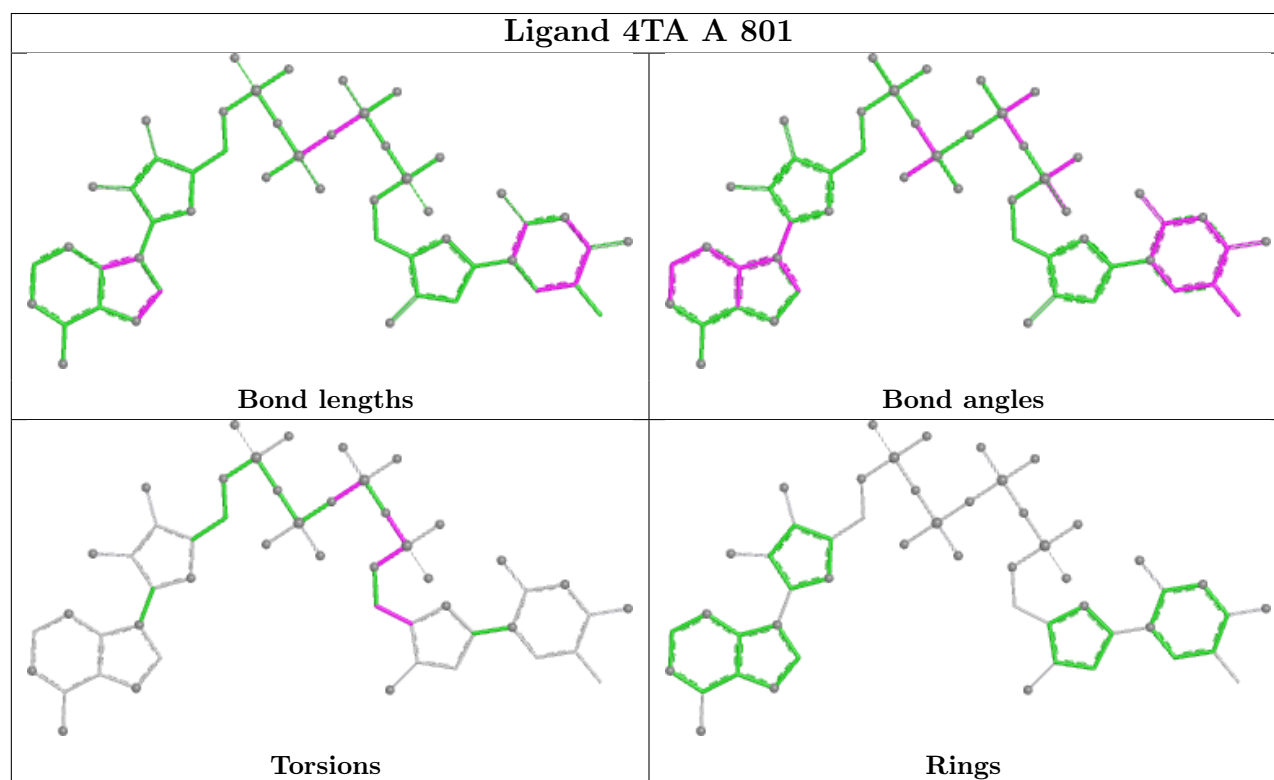
Mol	Chain	Res	Type	Atoms
3	A	801	4TA	C5B-O5'-PD-O2D
3	A	801	4TA	C5B-O5'-PD-O1D
3	A	801	4TA	C5B-O5'-PD-OCD
3	C	803	4TA	C5'-OA-PA-O2A
3	A	801	4TA	C3B-C4B-C5B-O5'
3	A	801	4TA	O4'-C4B-C5B-O5'
3	C	803	4TA	PC-OBC-PB-O1B
3	A	801	4TA	PC-OCD-PD-O5'
3	B	802	4TA	C5'-OA-PA-O2A
3	C	803	4TA	PA-OAB-PB-O2B
3	A	801	4TA	PB-OBC-PC-O2C
3	B	802	4TA	PA-OAB-PB-O2B
3	B	802	4TA	PA-OAB-PB-O1B
3	C	803	4TA	C2'-C1'-N9A-C8A
3	C	803	4TA	PA-OAB-PB-O1B
3	D	804	4TA	PB-OBC-PC-O2C

There are no ring outliers.

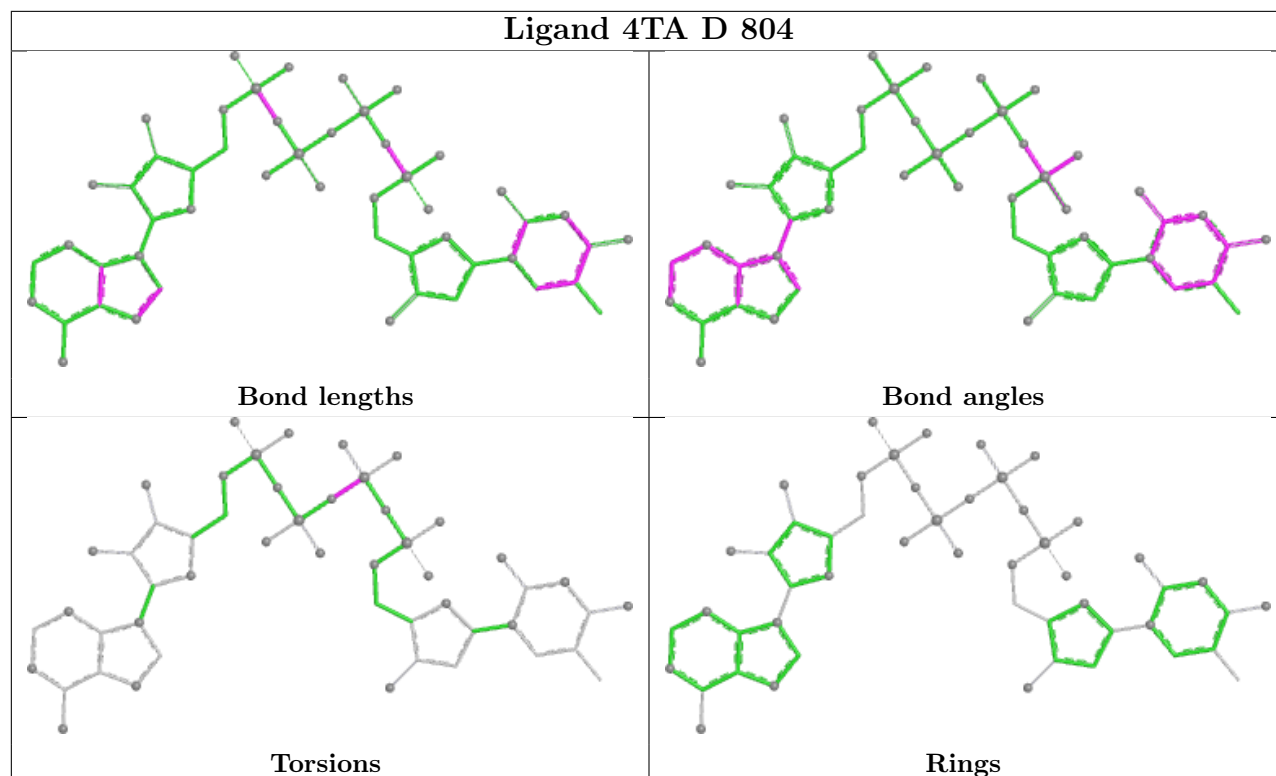
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	4TA	1	0
3	D	804	4TA	1	0
3	C	803	4TA	1	0
2	B	607	SO4	1	0
3	B	802	4TA	1	0

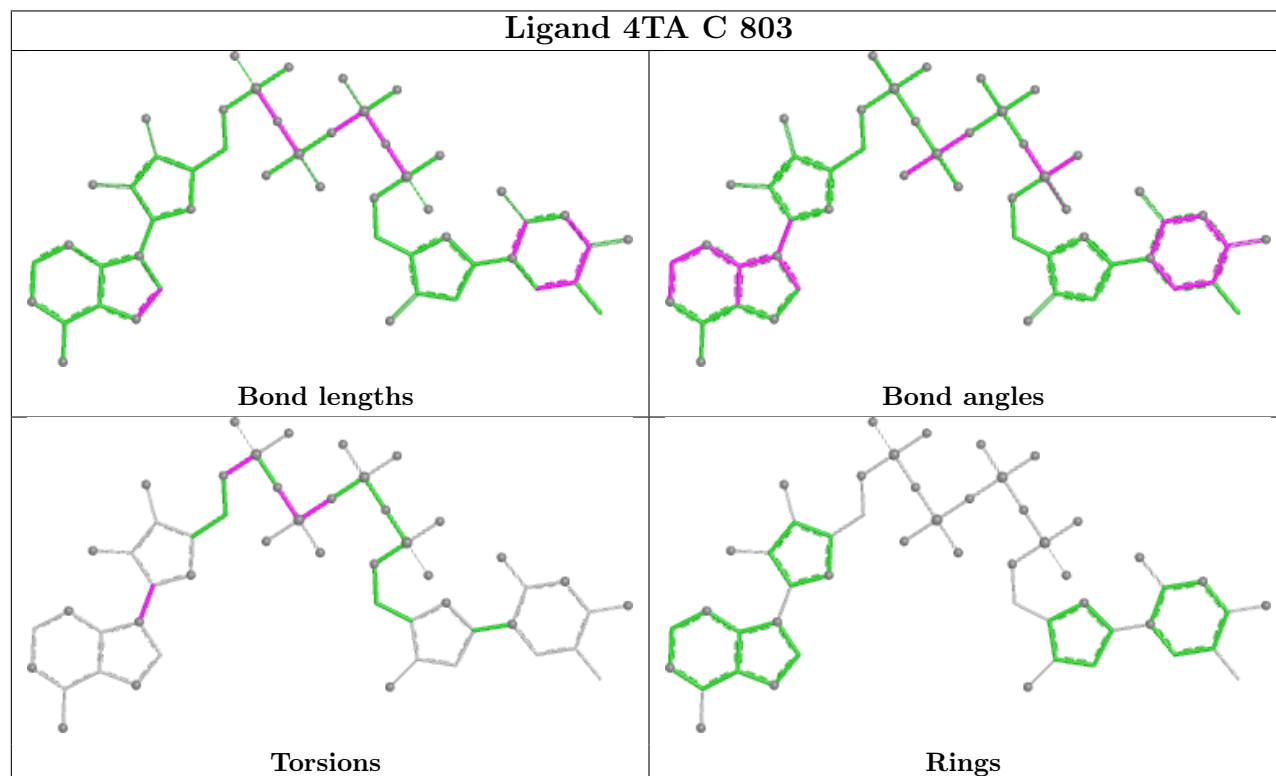
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

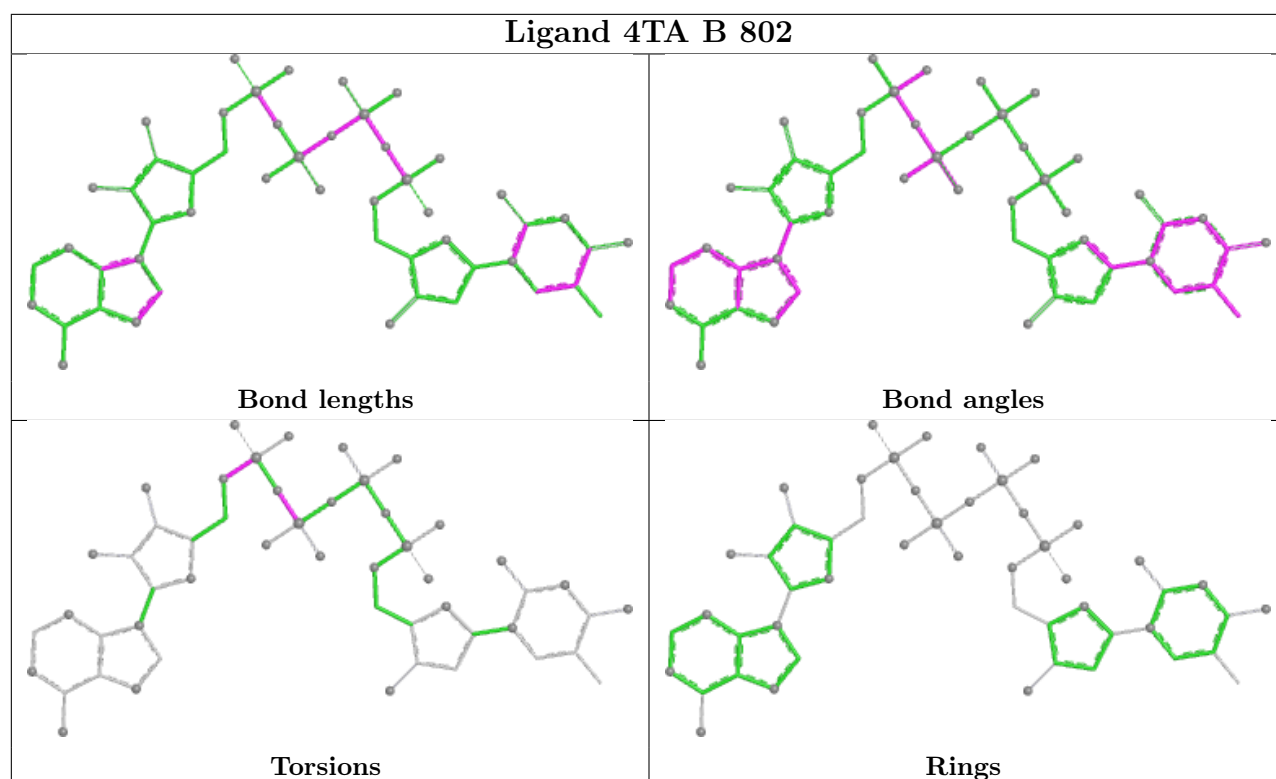


Ligand 4TA D 804



Ligand 4TA C 803





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/334 (95%)	0.46	23 (7%) 21 18	18, 33, 56, 68	1 (0%)
1	B	329/334 (98%)	0.45	37 (11%) 10 8	18, 33, 68, 80	0
1	C	317/334 (94%)	0.35	17 (5%) 31 27	19, 36, 54, 86	1 (0%)
1	D	326/334 (97%)	0.45	25 (7%) 19 17	23, 37, 56, 67	0
All	All	1292/1336 (96%)	0.43	102 (7%) 18 16	18, 35, 59, 86	2 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	ALA	20.7
1	A	151	ALA	12.8
1	C	197	ALA	7.3
1	C	352	VAL	6.6
1	B	91	VAL	5.3
1	A	152	ARG	5.1
1	B	89	LEU	5.0
1	B	78	TYR	4.9
1	B	82	ASN	4.3
1	B	88	ASN	4.3
1	B	77	ILE	4.2
1	A	82	ASN	4.1
1	D	82	ASN	4.1
1	B	95	ALA	4.0
1	B	83	ARG	3.9
1	D	352	VAL	3.9
1	C	92	ASP	3.9
1	A	79	ASP	3.7
1	B	74	ILE	3.6
1	A	163	LEU	3.6
1	D	83	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	202	GLN	3.6
1	B	81	GLN	3.5
1	B	86	GLN	3.5
1	B	75	SER	3.5
1	B	87	GLY	3.4
1	C	201	GLU	3.4
1	B	85	GLN	3.3
1	B	352	VAL	3.3
1	B	84	LYS	3.3
1	D	197	ALA	3.3
1	D	79	ASP	3.3
1	D	242	CYS	3.2
1	C	198	ARG	3.2
1	A	199	ILE	3.1
1	C	22	MET	3.1
1	B	244	ALA	3.0
1	D	78	TYR	3.0
1	A	92	ASP	3.0
1	B	76	GLY	3.0
1	C	247	HIS	3.0
1	C	279	ASP	2.9
1	D	77	ILE	2.9
1	A	200	GLY	2.9
1	B	199	ILE	2.9
1	B	73	VAL	2.8
1	D	81	GLN	2.8
1	B	90	ALA	2.8
1	B	79	ASP	2.8
1	A	157	ASP	2.8
1	B	94	ALA	2.8
1	C	262	GLU	2.8
1	B	196	ARG	2.8
1	B	102	GLN	2.7
1	D	21	HIS	2.7
1	A	240	THR	2.7
1	C	256	GLN	2.6
1	C	285	GLU	2.6
1	D	80	THR	2.6
1	C	253	ASP	2.6
1	C	91	VAL	2.6
1	B	195	THR	2.6
1	D	196	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	70	GLU	2.6
1	D	90	ALA	2.6
1	B	274	GLN	2.5
1	A	84	LYS	2.5
1	A	117	CYS	2.5
1	D	262	GLU	2.5
1	D	243	GLY	2.5
1	D	194	ARG	2.4
1	B	279	ASP	2.4
1	D	92	ASP	2.4
1	D	188	GLU	2.4
1	D	93	ASP	2.4
1	D	279	ASP	2.4
1	B	345	THR	2.3
1	A	53	SER	2.3
1	D	94	ALA	2.3
1	B	187	GLU	2.3
1	B	240	THR	2.3
1	D	74	ILE	2.2
1	D	75	SER	2.2
1	B	80	THR	2.2
1	A	242	CYS	2.2
1	B	241	SER	2.2
1	A	95	ALA	2.1
1	C	183	THR	2.1
1	A	340	GLU	2.1
1	A	22	MET	2.1
1	A	279	ASP	2.1
1	A	352	VAL	2.1
1	B	47	SER	2.1
1	D	195	THR	2.1
1	B	48	ALA	2.1
1	C	351	GLY	2.1
1	A	153	TYR	2.1
1	A	132	ASP	2.0
1	B	96	LEU	2.0
1	C	237	GLU	2.0
1	A	195	THR	2.0
1	B	194	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

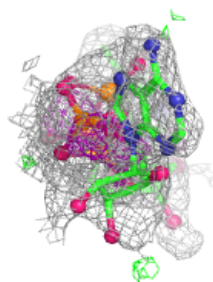
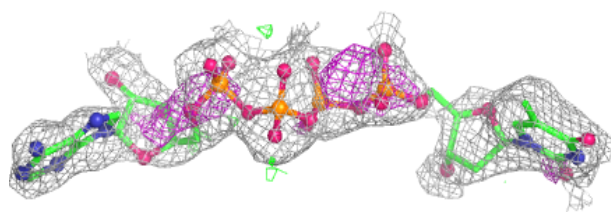
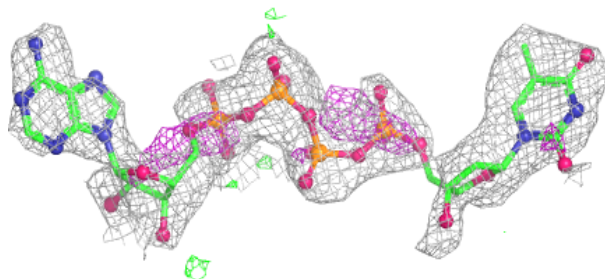
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	4TA	B	802	51/51	0.84	0.17	51,59,64,64	0
2	SO4	B	604	5/5	0.86	0.13	72,72,73,73	0
2	SO4	A	605	5/5	0.86	0.14	80,80,80,81	0
2	SO4	B	608	5/5	0.88	0.15	72,73,73,73	0
2	SO4	C	610	5/5	0.89	0.14	70,70,70,71	0
2	SO4	B	606	5/5	0.92	0.11	62,62,63,63	0
2	SO4	A	603	5/5	0.92	0.11	66,66,66,66	0
2	SO4	D	611	5/5	0.93	0.07	66,66,67,67	0
3	4TA	D	804	51/51	0.93	0.10	34,40,45,45	0
3	4TA	C	803	51/51	0.95	0.08	26,41,46,47	0
2	SO4	A	601	5/5	0.96	0.09	46,47,49,49	0
2	SO4	C	609	5/5	0.96	0.10	51,51,53,53	0
3	4TA	A	801	51/51	0.96	0.07	24,37,43,44	0
2	SO4	A	602	5/5	0.97	0.09	37,39,39,40	0
2	SO4	B	607	5/5	0.98	0.10	41,41,42,42	0

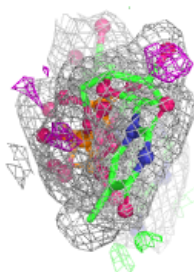
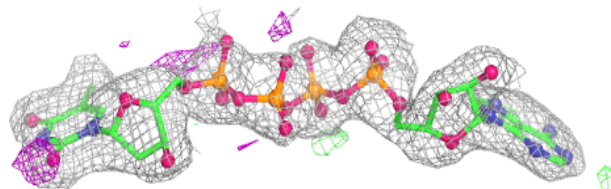
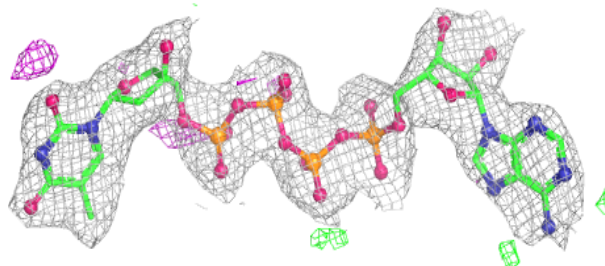
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4TA B 802:

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

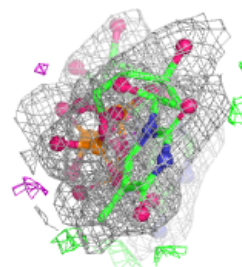
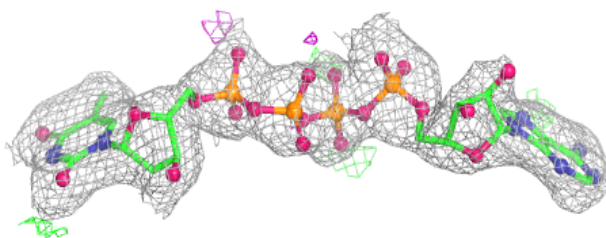
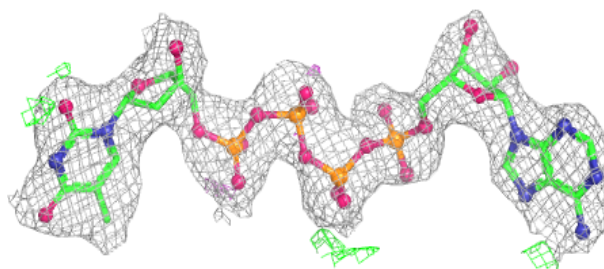
**Electron density around 4TA D 804:**

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

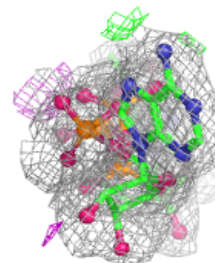
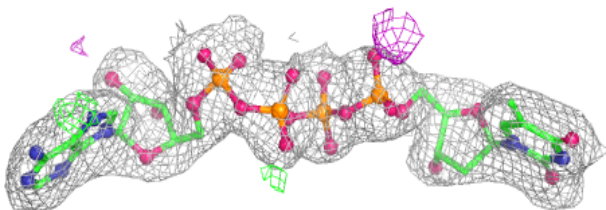
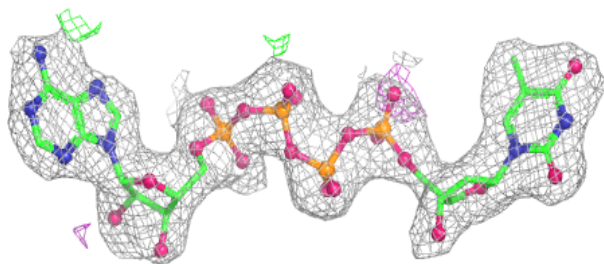


Electron density around 4TA C 803:

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

**Electron density around 4TA A 801:**

$2mF_o-DF_c$ (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.