Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 07:04 PM EDT

PDB ID	:	1P75
Title	:	Crystal structure of EHV4-TK complexed with TP5A
Authors	:	Gardberg, A.; Shuvalova, L.; Monnerjahn, C.; Konrad, M.; Lavie, A.
Deposited on	:	2003-04-30
Resolution	:	3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

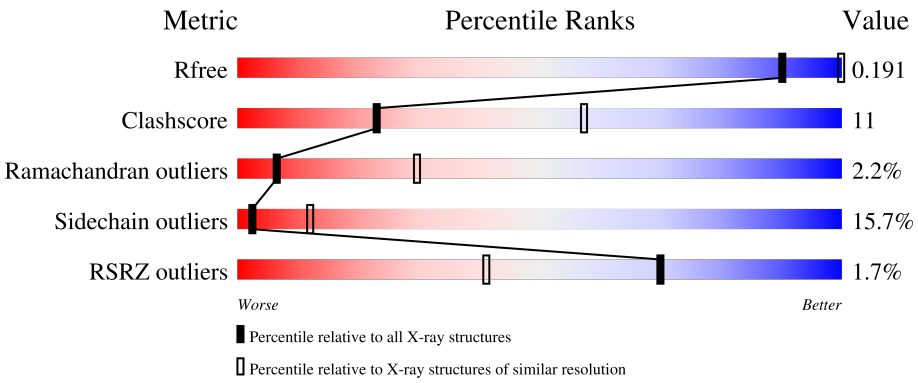
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	2% 65% 28% 7% •
1	B	334	% 67% 26% 6% •
1	C	334	% 64% 28% 6% •
1	D	334	3% 68% 25% 5% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10704 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.

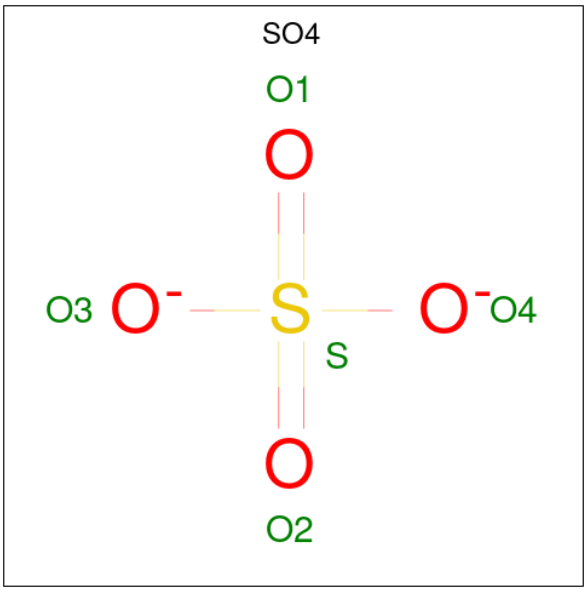
- Molecule 1 is a protein called Thymidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2540	1606	444	472	18	0	0	0
1	B	333	2564	1617	451	478	18	0	0	0
1	C	330	2548	1609	444	477	18	0	0	0
1	D	328	2505	1587	435	465	18	0	0	0

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 (three-letter code: SO4) (formula: O_4S).



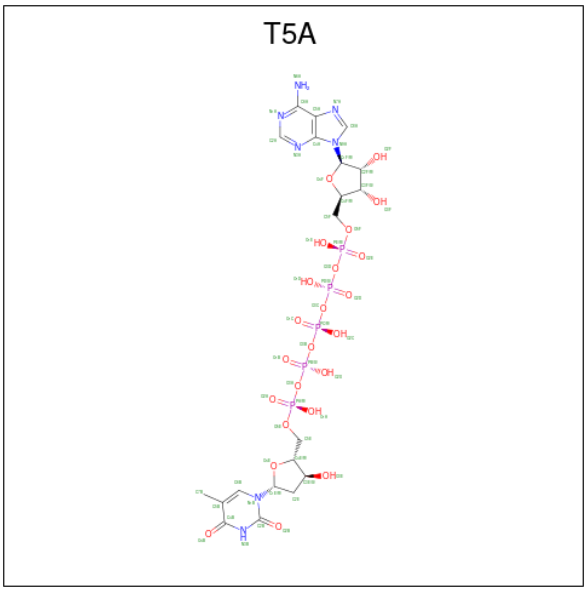
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is P1-(5'-ADENOSYL)P5-(5'-THYMIDYL)PENTAPHOSPHATE (three-letter code: T5A) (formula: $C_{20}H_{30}N_7O_{23}P_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	78	22	7	39	10	0	1
			Total	C	N	O	P		
3	B	1	78	22	7	39	10	0	1
			Total	C	N	O	P		
3	C	1	78	22	7	39	10	0	1
			Total	C	N	O	P		
3	D	1	78	22	7	39	10	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	46	46	46	0	0
			Total	O		
4	B	24	24	24	0	0
			Total	O		
4	C	43	43	43	0	0

Continued on next page...

Continued from previous page...

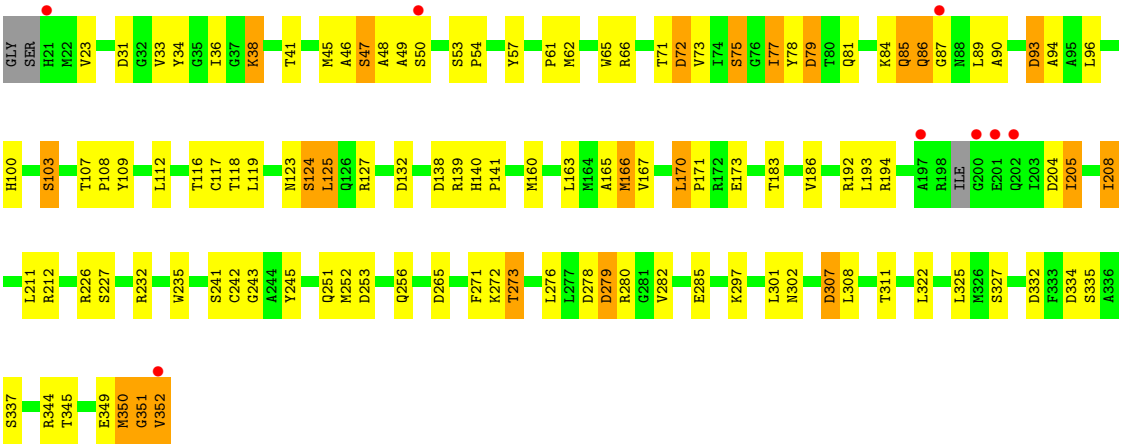
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	42	42	42	0	0

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.

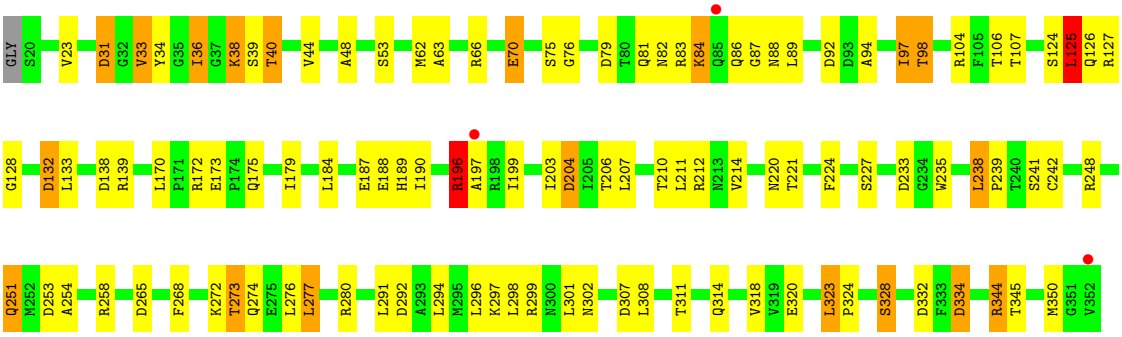
• Molecule 1: Thymidine kinase

Chain A:



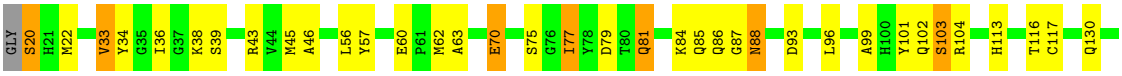
• Molecule 1: Thymidine kinase

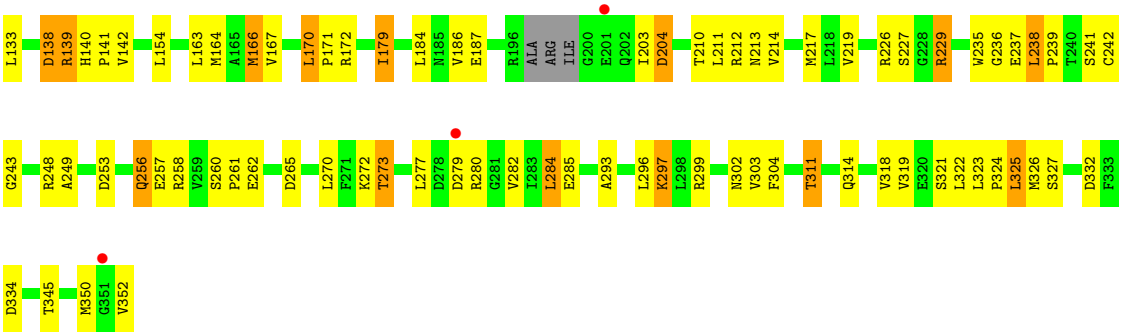
Chain B:



• Molecule 1: Thymidine kinase

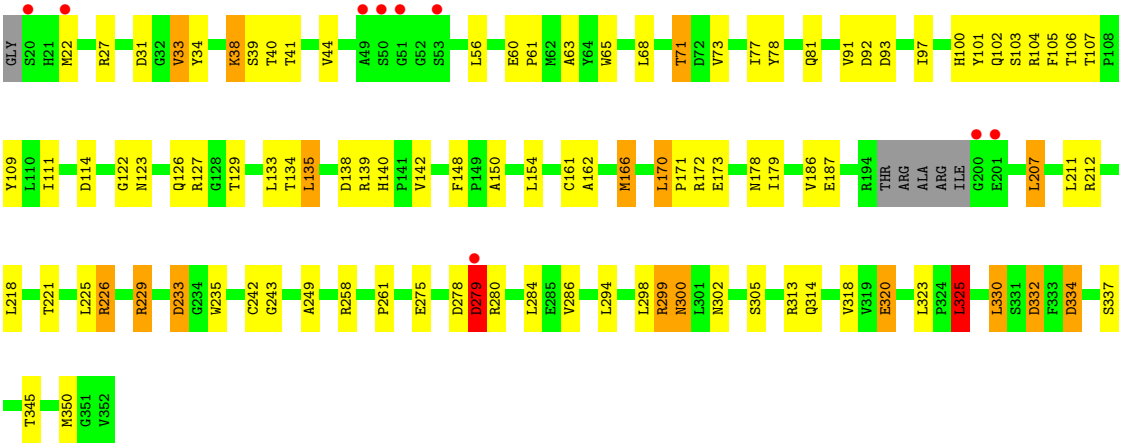
Chain C:





- Molecule 1: Thymidine kinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.87Å 117.23Å 125.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 3.02 29.58 – 3.02	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.58-3.02) 97.0 (29.58-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.38 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.298 0.203 , 0.191	Depositor DCC
R_{free} test set	3105 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10704	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: T5A, SO4

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	0.60	0/2591	0.85	11/3523 (0.3%)
1	B	0.59	0/2616	0.86	9/3557 (0.3%)
1	C	0.59	0/2600	0.86	7/3534 (0.2%)
1	D	0.56	0/2556	0.84	7/3478 (0.2%)
All	All	0.59	0/10363	0.85	34/14092 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ASP	CB-CG-OD2	7.61	125.15	118.30
1	B	253	ASP	CB-CG-OD2	7.12	124.71	118.30
1	C	279	ASP	CB-CG-OD2	6.65	124.29	118.30
1	C	284	LEU	CA-CB-CG	6.54	130.34	115.30
1	A	79	ASP	CB-CG-OD2	6.31	123.97	118.30
1	B	132	ASP	CB-CG-OD2	6.26	123.93	118.30
1	D	332	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	204	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	265	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	278	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	79	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	125	LEU	CA-CB-CG	5.95	128.98	115.30
1	C	332	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	132	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	334	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	114	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	279	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	31	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	93	ASP	CB-CG-OD2	5.55	123.29	118.30
1	D	233	ASP	CB-CG-OD2	5.55	123.29	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	93	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	92	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	233	ASP	CB-CG-OD2	5.36	123.13	118.30
1	B	332	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	334	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	334	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	265	ASP	CB-CG-OD2	5.27	123.05	118.30
1	C	138	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	93	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	292	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	334	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	325	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	117	CYS	CA-CB-SG	-5.18	104.67	114.00
1	B	307	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2540	0	2497	60	0
1	B	2564	0	2533	57	0
1	C	2548	0	2510	67	0
1	D	2505	0	2454	50	0
2	A	25	0	0	1	0
2	B	35	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
3	A	78	0	12	5	0
3	B	78	0	12	7	0
3	C	78	0	12	5	0
3	D	78	0	12	6	0
4	A	46	0	0	1	0
4	B	24	0	0	1	0
4	C	43	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	42	0	0	4	0
All	All	10704	0	10042	236	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 (236) 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:34:TYR:HB2	3:A:501[B]:T5A:O2X	1.59	1.03
1:B:344:ARG:HG2	1:B:344:ARG:HH11	1.28	0.97
1:C:34:TYR:HB2	3:C:503[B]:T5A:O2X	1.68	0.93
1:B:34:TYR:HB2	3:B:502[B]:T5A:O2X	1.70	0.91
1:C:238:LEU:HD12	1:C:239:PRO:HD2	1.51	0.91
1:A:61:PRO:HA	1:A:350:MET:HG3	1.53	0.90
1:D:173:GLU:O	1:D:300:ASN:ND2	2.09	0.85
1:C:242:CYS:HA	4:C:755:HOH:O	1.75	0.85
1:C:229:ARG:NH2	1:C:261:PRO:O	2.11	0.84
1:B:311:THR:H	1:B:314:GLN:HG3	1.43	0.83
1:C:87:GLY:O	1:C:88:ASN:HB2	1.79	0.82
1:A:46:ALA:HB2	1:A:57:TYR:HB2	1.65	0.79
3:B:502[B]:T5A:O1C	3:B:502[B]:T5A:O2E	2.03	0.76
1:B:39:SER:HB2	3:B:502[B]:T5A:O1D	1.84	0.76
1:C:226:ARG:HD2	4:C:721:HOH:O	1.83	0.76
1:C:179:ILE:HG23	1:C:303:VAL:HG22	1.69	0.74
1:B:274:GLN:HA	1:B:277:LEU:HD12	1.69	0.74
1:B:251:GLN:HG2	1:B:254:ALA:HB2	1.68	0.74
1:B:196:ARG:NH1	3:B:502[B]:T5A:O2C	2.21	0.73
1:D:73:VAL:HG13	4:D:753:HOH:O	1.92	0.70
1:A:138:ASP:O	1:A:139:ARG:HB2	1.90	0.69
1:C:164:MET:HE1	4:C:738:HOH:O	1.93	0.69
1:A:232:ARG:HG2	1:A:232:ARG:HH11	1.60	0.67
1:A:53:SER:HB3	1:A:54:PRO:HD2	1.77	0.66
3:A:501[A]:T5A:O2C	3:A:501[A]:T5A:O2A	2.14	0.65
1:D:154:LEU:HD13	1:D:249:ALA:HB1	1.77	0.65
1:C:210:THR:O	1:C:214:VAL:HG23	1.96	0.65
1:B:203:ILE:O	1:B:204:ASP:HB3	1.98	0.64
1:A:256:GLN:HB2	4:A:741:HOH:O	1.96	0.64
1:C:113:HIS:CE1	1:C:117:CYS:SG	2.90	0.64
3:D:504[A]:T5A:O2X	4:D:736:HOH:O	2.14	0.64
1:A:112:LEU:O	1:A:116:THR:HG23	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLY:O	1:C:88:ASN:CB	2.46	0.63
1:B:40:THR:O	1:B:44:VAL:HG23	1.99	0.63
1:D:33:VAL:HG21	1:D:212:ARG:HG3	1.80	0.63
1:C:63:ALA:HB3	1:C:350:MET:HA	1.79	0.63
1:C:213:ASN:O	1:C:217:MET:HG3	1.99	0.62
1:A:72:ASP:OD1	1:A:75:SER:HB3	1.99	0.62
1:C:323:LEU:HD12	1:C:326:MET:HE3	1.82	0.62
1:A:235:TRP:CZ2	1:A:272:LYS:HG3	2.35	0.61
1:D:150:ALA:O	1:D:154:LEU:HG	2.01	0.60
1:C:311:THR:HG23	1:C:314:GLN:OE1	2.01	0.60
1:D:279:ASP:OD1	1:D:279:ASP:N	2.25	0.60
1:A:170:LEU:HD23	1:A:171:PRO:HD2	1.82	0.60
1:B:173:GLU:HG2	1:B:301:LEU:HD23	1.83	0.59
1:D:314:GLN:O	1:D:318:VAL:HG23	2.02	0.59
1:B:38:LYS:NZ	3:B:502[A]:T5A:O2C	2.36	0.59
1:A:140:HIS:NE2	1:A:173:GLU:OE1	2.35	0.58
1:B:94:ALA:O	1:B:98:THR:HB	2.03	0.58
1:C:45:MET:CE	1:C:319:VAL:HB	2.34	0.58
1:C:46:ALA:HB2	1:C:57:TYR:HB2	1.85	0.58
1:D:221:THR:O	1:D:225:LEU:HG	2.04	0.58
1:C:138:ASP:O	1:C:139:ARG:HB2	2.03	0.58
1:D:71:THR:HB	2:D:713:SO4:O1	2.03	0.58
1:C:226:ARG:NH2	1:C:303:VAL:H	2.01	0.57
1:B:311:THR:OG1	1:B:314:GLN:HG3	2.04	0.57
1:B:311:THR:N	1:B:314:GLN:HG3	2.17	0.57
1:D:140:HIS:HB3	1:D:142:VAL:HG12	1.87	0.56
1:A:36:ILE:HG23	1:A:308:LEU:HD12	1.86	0.56
1:C:237:GLU:CD	1:C:237:GLU:H	2.08	0.56
1:D:278:ASP:HB3	1:D:284:LEU:HD21	1.86	0.56
1:D:229:ARG:NH2	1:D:261:PRO:O	2.36	0.56
1:A:232:ARG:HG2	1:A:232:ARG:NH1	2.20	0.56
1:D:60:GLU:HG2	1:D:109:TYR:OH	2.05	0.55
1:D:38:LYS:NZ	3:D:504[A]:T5A:O2C	2.38	0.55
1:C:33:VAL:HG13	1:C:211:LEU:HB3	1.88	0.55
1:A:124:SER:O	1:A:125:LEU:HD23	2.06	0.55
1:B:172:ARG:HA	1:B:297:LYS:HG2	1.87	0.55
1:C:226:ARG:HH22	1:C:303:VAL:H	1.54	0.55
1:A:62:MET:O	1:A:66:ARG:HG3	2.07	0.54
1:B:83:ARG:HH21	1:B:89:LEU:HD13	1.70	0.54
1:B:203:ILE:O	1:B:204:ASP:CB	2.56	0.54
1:C:20:SER:N	4:C:727:HOH:O	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:GLU:CD	1:C:237:GLU:N	2.61	0.54
1:D:148:PHE:CE2	1:D:211:LEU:HD11	2.42	0.54
1:B:36:ILE:HG13	1:B:189:HIS:CE1	2.43	0.54
1:A:53:SER:HB3	1:A:54:PRO:CD	2.37	0.54
1:D:294:LEU:O	1:D:298:LEU:HG	2.07	0.54
1:B:48:ALA:HB1	1:C:133:LEU:HD13	1.90	0.54
1:D:226:ARG:NH2	4:D:733:HOH:O	2.40	0.54
1:B:63:ALA:HB3	1:B:350:MET:HA	1.90	0.53
1:D:133:LEU:HD12	1:D:134:THR:H	1.73	0.53
1:D:73:VAL:HG11	1:D:104:ARG:HB3	1.89	0.53
1:B:33:VAL:HG21	1:B:212:ARG:HG2	1.91	0.53
1:C:235:TRP:CE2	1:C:272:LYS:HD2	2.43	0.53
1:D:187:GLU:OE1	1:D:187:GLU:HA	2.09	0.53
1:D:320:GLU:O	1:D:323:LEU:HB2	2.09	0.53
1:A:119:LEU:HB3	1:A:335:SER:HB3	1.91	0.53
1:B:138:ASP:O	1:B:139:ARG:HB2	2.09	0.53
1:B:344:ARG:HG2	1:B:344:ARG:NH1	2.04	0.53
1:C:81:GLN:O	1:C:85:GLN:HG3	2.09	0.53
1:B:210:THR:O	1:B:214:VAL:HG23	2.09	0.52
3:C:503[A]:T5A:O2C	3:C:503[A]:T5A:O2A	2.28	0.52
1:D:170:LEU:HD23	1:D:171:PRO:HD2	1.91	0.52
1:D:162:ALA:O	1:D:166:MET:HG2	2.09	0.52
1:A:36:ILE:N	3:A:501[A]:T5A:O1D	2.43	0.52
3:D:504[B]:T5A:O1C	3:D:504[B]:T5A:O2E	2.27	0.52
1:C:314:GLN:O	1:C:318:VAL:HG23	2.10	0.52
1:D:138:ASP:O	1:D:139:ARG:HB2	2.10	0.52
1:B:124:SER:HA	1:B:328:SER:O	2.10	0.51
1:A:100:HIS:O	1:A:103:SER:HB2	2.10	0.51
1:A:241:SER:O	1:A:273:THR:HG23	2.10	0.51
1:C:104:ARG:HD3	1:D:161:CYS:SG	2.51	0.51
1:A:90:ALA:HB3	1:A:93:ASP:HB2	1.92	0.51
1:D:107:THR:O	1:D:111:ILE:HG13	2.11	0.51
1:D:34:TYR:HB2	3:D:504[B]:T5A:O2X	2.11	0.51
1:B:31:ASP:OD2	1:B:139:ARG:NH1	2.43	0.50
1:C:203:ILE:O	1:C:204:ASP:CB	2.59	0.50
1:A:62:MET:SD	1:A:66:ARG:HD2	2.51	0.50
1:A:241:SER:HB3	1:A:245:TYR:CD2	2.46	0.50
1:D:33:VAL:HG21	1:D:212:ARG:CG	2.42	0.50
1:B:179:ILE:HG22	1:B:301:LEU:HB3	1.93	0.49
1:A:89:LEU:O	1:A:90:ALA:C	2.51	0.49
1:A:96:LEU:HB2	1:B:97:ILE:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:HIS:CD2	1:C:141:PRO:HD2	2.48	0.49
1:D:27:ARG:HB3	1:D:135:LEU:HD12	1.93	0.49
1:D:27:ARG:O	1:D:178:ASN:HB2	2.13	0.49
1:C:33:VAL:HG21	1:C:212:ARG:HG2	1.94	0.49
1:A:65:TRP:HH2	1:A:109:TYR:HH	1.60	0.49
1:C:203:ILE:O	1:C:204:ASP:HB3	2.12	0.49
1:B:70:GLU:HA	1:B:70:GLU:OE1	2.13	0.49
1:B:224:PHE:O	1:B:227:SER:HB2	2.13	0.48
1:A:140:HIS:CG	1:A:141:PRO:HD2	2.47	0.48
1:D:334:ASP:O	1:D:337:SER:HB2	2.12	0.48
1:C:304:PHE:CD2	1:C:322:LEU:HD22	2.49	0.48
1:B:311:THR:HG23	1:B:314:GLN:HE21	1.78	0.48
1:C:45:MET:HE1	1:C:319:VAL:HB	1.95	0.48
1:A:163:LEU:O	1:A:167:VAL:HG23	2.14	0.48
1:C:39:SER:HB2	3:C:503[B]:T5A:O1D	2.14	0.48
1:C:256:GLN:HB3	4:C:750:HOH:O	2.14	0.48
1:C:63:ALA:CB	1:C:350:MET:HA	2.44	0.47
1:A:61:PRO:CA	1:A:350:MET:HG3	2.33	0.47
1:B:314:GLN:O	1:B:318:VAL:HG23	2.14	0.47
1:C:70:GLU:HB2	2:C:715:SO4:O1	2.14	0.47
1:C:62:MET:HG2	1:C:352:VAL:HG21	1.96	0.47
1:A:170:LEU:O	1:A:297:LYS:HD3	2.15	0.47
1:B:221:THR:O	1:B:224:PHE:HB3	2.15	0.47
1:C:103:SER:HA	1:C:166:MET:HE1	1.95	0.47
1:A:285:GLU:HB3	1:B:345:THR:HG21	1.96	0.47
1:C:163:LEU:O	1:C:167:VAL:HG23	2.15	0.46
1:A:242:CYS:O	1:A:245:TYR:N	2.49	0.46
1:C:39:SER:N	3:C:503[A]:T5A:O2D	2.40	0.46
1:A:208:ILE:O	1:A:212:ARG:HG3	2.15	0.46
1:B:241:SER:O	1:B:273:THR:HG23	2.15	0.46
1:B:33:VAL:HG13	1:B:211:LEU:HB3	1.97	0.46
1:C:140:HIS:HB3	1:C:142:VAL:HG12	1.96	0.46
1:A:349:GLU:C	1:A:351:GLY:H	2.19	0.46
1:B:235:TRP:CZ2	1:B:272:LYS:HG3	2.51	0.45
1:D:278:ASP:HB3	1:D:284:LEU:CD2	2.46	0.45
1:B:125:LEU:O	1:B:127:ARG:HG3	2.16	0.45
1:C:36:ILE:N	3:C:503[A]:T5A:O1D	2.49	0.45
1:C:323:LEU:N	1:C:324:PRO:HD2	2.31	0.45
1:A:170:LEU:CD2	1:A:171:PRO:HD2	2.44	0.45
1:A:183:THR:O	1:A:307:ASP:HA	2.16	0.45
1:C:184:LEU:HD12	1:C:184:LEU:HA	1.74	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:CYS:HB2	4:C:736:HOH:O	2.16	0.45
3:D:504[B]:T5A:O3C	3:D:504[B]:T5A:HA52	2.16	0.45
1:D:127:ARG:HH21	1:D:330:LEU:HD21	1.81	0.45
1:D:127:ARG:NH2	1:D:330:LEU:HD21	2.32	0.45
1:A:271:PHE:O	1:A:276:LEU:HD12	2.17	0.45
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.82	0.45
1:B:173:GLU:HG2	1:B:301:LEU:CD2	2.47	0.45
1:B:82:ASN:O	1:B:86:GLN:HB2	2.17	0.44
1:A:36:ILE:O	1:A:192:ARG:NH1	2.51	0.44
1:D:207:LEU:HD21	4:D:738:HOH:O	2.18	0.44
1:A:205:ILE:H	1:A:205:ILE:HG12	1.52	0.44
1:B:83:ARG:NH2	1:B:89:LEU:HD13	2.32	0.44
1:A:47:SER:C	1:A:49:ALA:H	2.21	0.44
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.89	0.43
1:D:65:TRP:O	1:D:73:VAL:HG22	2.19	0.43
3:A:501[B]:T5A:O1C	3:A:501[B]:T5A:O2E	2.37	0.43
1:D:33:VAL:HG13	1:D:211:LEU:HB3	2.00	0.43
1:D:63:ALA:HB3	1:D:350:MET:HA	2.00	0.43
1:C:45:MET:HE3	1:C:319:VAL:HB	2.00	0.43
1:B:268:PHE:CE1	1:B:294:LEU:HD23	2.53	0.43
1:C:241:SER:O	1:C:273:THR:HG23	2.18	0.43
1:A:41:THR:O	1:A:45:MET:HG3	2.18	0.43
1:B:36:ILE:N	3:B:502[A]:T5A:O1D	2.51	0.43
1:B:323:LEU:N	1:B:324:PRO:HD2	2.34	0.43
1:A:350:MET:O	1:A:351:GLY:O	2.37	0.43
1:C:75:SER:O	1:C:79:ASP:HB2	2.19	0.43
1:D:102:GLN:O	1:D:105:PHE:HB2	2.19	0.43
1:D:122:GLY:O	1:D:123:ASN:HB2	2.19	0.43
1:A:107:THR:HB	1:A:108:PRO:CD	2.49	0.43
1:C:166:MET:O	1:C:167:VAL:C	2.57	0.43
1:A:33:VAL:HG21	1:A:212:ARG:HG2	2.01	0.43
1:A:351:GLY:O	1:A:352:VAL:C	2.57	0.42
1:C:170:LEU:HD22	1:C:171:PRO:HD2	2.00	0.42
1:A:71:THR:N	2:A:708:SO4:O3	2.52	0.42
1:B:220:ASN:HD22	1:B:265:ASP:HB3	1.83	0.42
1:C:235:TRP:O	1:C:236:GLY:C	2.57	0.42
1:B:36:ILE:HG22	1:B:308:LEU:HD12	2.02	0.42
1:B:48:ALA:HB1	1:C:133:LEU:CD1	2.48	0.42
1:A:211:LEU:HA	1:A:211:LEU:HD23	1.73	0.42
1:D:103:SER:HA	1:D:166:MET:HE1	2.02	0.42
1:A:85:GLN:C	1:A:87:GLY:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:MET:HE2	1:A:166:MET:HB3	1.98	0.42
1:A:77:ILE:HG22	1:A:78:TYR:N	2.35	0.42
1:A:103:SER:HA	1:A:166:MET:HE1	2.01	0.42
1:A:47:SER:O	1:A:49:ALA:N	2.52	0.42
1:B:23:VAL:HA	1:B:132:ASP:OD2	2.20	0.42
1:B:39:SER:N	3:B:502[A]:T5A:O2D	2.33	0.42
1:C:113:HIS:CE1	1:C:117:CYS:HG	2.37	0.42
1:C:293:ALA:O	1:C:297:LYS:HB2	2.20	0.42
1:B:184:LEU:HD23	1:B:189:HIS:HA	2.01	0.42
1:A:38:LYS:HG2	3:A:501[A]:T5A:O2D	2.20	0.41
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.89	0.41
1:A:165:ALA:HA	1:B:107:THR:OG1	2.20	0.41
1:B:188:GLU:HA	1:B:188:GLU:OE1	2.19	0.41
1:C:323:LEU:HA	1:C:326:MET:HG3	2.01	0.41
1:B:124:SER:HB3	1:B:175:GLN:HB2	2.02	0.41
1:C:99:ALA:HB1	1:D:100:HIS:CE1	2.56	0.41
1:C:323:LEU:HA	1:C:326:MET:HE2	2.03	0.41
1:A:85:GLN:O	1:A:87:GLY:N	2.44	0.41
1:A:123:ASN:O	1:A:127:ARG:NH2	2.39	0.41
1:C:77:ILE:HG12	1:C:101:TYR:HB3	2.03	0.41
1:D:127:ARG:C	1:D:129:THR:H	2.24	0.41
1:C:154:LEU:HD22	1:C:249:ALA:HB3	2.03	0.41
1:C:241:SER:O	1:C:273:THR:CG2	2.68	0.41
1:C:319:VAL:O	1:C:322:LEU:HB2	2.21	0.41
1:C:325:LEU:HD12	1:C:325:LEU:HA	1.82	0.41
1:D:61:PRO:HA	1:D:350:MET:HB3	2.02	0.41
1:D:73:VAL:HG12	1:D:101:TYR:HD2	1.86	0.41
1:D:325:LEU:N	1:D:325:LEU:HD23	2.35	0.41
1:A:100:HIS:CD2	1:A:100:HIS:C	2.95	0.40
1:A:84:LYS:HB2	1:A:94:ALA:CB	2.52	0.40
1:B:207:LEU:HG	1:B:211:LEU:HD12	2.03	0.40
1:B:238:LEU:HA	1:B:239:PRO:HD3	1.85	0.40
1:B:179:ILE:CG2	1:B:301:LEU:HB3	2.52	0.40
1:C:172:ARG:HG3	1:C:172:ARG:NH1	2.37	0.40
1:D:40:THR:O	1:D:41:THR:C	2.58	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	327/334 (98%)	303 (93%)	20 (6%)	4 (1%)	13 46
1	B	331/334 (99%)	297 (90%)	22 (7%)	12 (4%)	3 18
1	C	326/334 (98%)	295 (90%)	27 (8%)	4 (1%)	13 46
1	D	324/334 (97%)	297 (92%)	18 (6%)	9 (3%)	5 24
All	All	1308/1336 (98%)	1192 (91%)	87 (7%)	29 (2%)	6 30

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	GLY
1	B	88	ASN
1	B	196	ARG
1	C	88	ASN
1	C	204	ASP
1	D	22	MET
1	D	243	GLY
1	A	48	ALA
1	A	86	GLN
1	B	76	GLY
1	B	87	GLY
1	B	128	GLY
1	B	197	ALA
1	B	204	ASP
1	C	243	GLY
1	D	91	VAL
1	D	233	ASP
1	A	243	GLY
1	B	84	LYS
1	B	126	GLN
1	D	299	ARG
1	B	75	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	298	LEU
1	D	235	TRP
1	D	300	ASN
1	C	139	ARG
1	D	242	CYS
1	D	279	ASP
1	B	199	ILE

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	268/279 (96%)	224 (84%)	44 (16%)	2 11
1	B	274/279 (98%)	234 (85%)	40 (15%)	3 14
1	C	273/279 (98%)	225 (82%)	48 (18%)	2 9
1	D	263/279 (94%)	226 (86%)	37 (14%)	3 15
All	All	1078/1116 (97%)	909 (84%)	169 (16%)	2 12

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	38	LYS
1	A	47	SER
1	A	50	SER
1	A	73	VAL
1	A	75	SER
1	A	77	ILE
1	A	79	ASP
1	A	81	GLN
1	A	85	GLN
1	A	86	GLN
1	A	103	SER
1	A	118	THR
1	A	124	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	125	LEU
1	A	160	MET
1	A	166	MET
1	A	170	LEU
1	A	186	VAL
1	A	193	LEU
1	A	194	ARG
1	A	205	ILE
1	A	208	ILE
1	A	226	ARG
1	A	227	SER
1	A	251	GLN
1	A	252	MET
1	A	253	ASP
1	A	273	THR
1	A	279	ASP
1	A	280	ARG
1	A	282	VAL
1	A	302	ASN
1	A	307	ASP
1	A	311	THR
1	A	322	LEU
1	A	325	LEU
1	A	327	SER
1	A	332	ASP
1	A	337	SER
1	A	344	ARG
1	A	345	THR
1	A	350	MET
1	A	352	VAL
1	B	31	ASP
1	B	33	VAL
1	B	36	ILE
1	B	38	LYS
1	B	40	THR
1	B	53	SER
1	B	62	MET
1	B	66	ARG
1	B	70	GLU
1	B	81	GLN
1	B	84	LYS
1	B	92	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	97	ILE
1	B	98	THR
1	B	104	ARG
1	B	106	THR
1	B	125	LEU
1	B	133	LEU
1	B	170	LEU
1	B	187	GLU
1	B	190	ILE
1	B	196	ARG
1	B	206	THR
1	B	238	LEU
1	B	242	CYS
1	B	248	ARG
1	B	251	GLN
1	B	258	ARG
1	B	273	THR
1	B	276	LEU
1	B	277	LEU
1	B	280	ARG
1	B	296	LEU
1	B	299	ARG
1	B	302	ASN
1	B	320	GLU
1	B	323	LEU
1	B	328	SER
1	B	334	ASP
1	B	344	ARG
1	C	20	SER
1	C	22	MET
1	C	33	VAL
1	C	38	LYS
1	C	43	ARG
1	C	60	GLU
1	C	70	GLU
1	C	77	ILE
1	C	81	GLN
1	C	84	LYS
1	C	86	GLN
1	C	96	LEU
1	C	102	GLN
1	C	103	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	116	THR
1	C	130	GLN
1	C	166	MET
1	C	170	LEU
1	C	179	ILE
1	C	186	VAL
1	C	187	GLU
1	C	219	VAL
1	C	227	SER
1	C	229	ARG
1	C	238	LEU
1	C	248	ARG
1	C	253	ASP
1	C	256	GLN
1	C	257	GLU
1	C	258	ARG
1	C	260	SER
1	C	262	GLU
1	C	270	LEU
1	C	273	THR
1	C	277	LEU
1	C	280	ARG
1	C	282	VAL
1	C	284	LEU
1	C	285	GLU
1	C	296	LEU
1	C	297	LYS
1	C	299	ARG
1	C	302	ASN
1	C	311	THR
1	C	321	SER
1	C	325	LEU
1	C	327	SER
1	C	345	THR
1	D	31	ASP
1	D	33	VAL
1	D	38	LYS
1	D	39	SER
1	D	44	VAL
1	D	56	LEU
1	D	68	LEU
1	D	71	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	77	ILE
1	D	81	GLN
1	D	97	ILE
1	D	106	THR
1	D	126	GLN
1	D	135	LEU
1	D	166	MET
1	D	170	LEU
1	D	172	ARG
1	D	179	ILE
1	D	186	VAL
1	D	207	LEU
1	D	218	LEU
1	D	226	ARG
1	D	229	ARG
1	D	258	ARG
1	D	275	GLU
1	D	279	ASP
1	D	280	ARG
1	D	286	VAL
1	D	299	ARG
1	D	302	ASN
1	D	305	SER
1	D	313	ARG
1	D	320	GLU
1	D	325	LEU
1	D	330	LEU
1	D	332	ASP
1	D	345	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	123	ASN
1	A	302	ASN
1	B	189	HIS
1	B	287	HIS
1	B	300	ASN
1	B	302	ASN
1	B	314	GLN
1	C	130	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	202	GLN
1	C	251	GLN
1	C	302	ASN
1	D	302	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	T5A	C	503[A]	-	48,59,59	1.28	4 (8%)	59,93,93	1.96	12 (20%)
2	SO4	B	710	-	4,4,4	0.14	0	6,6,6	0.36	0
3	T5A	D	504[A]	-	48,59,59	1.32	7 (14%)	59,93,93	2.04	13 (22%)
2	SO4	A	708	-	4,4,4	0.13	0	6,6,6	0.42	0
3	T5A	B	502[B]	-	48,59,59	1.29	9 (18%)	59,93,93	2.06	16 (27%)
2	SO4	A	702	-	4,4,4	0.17	0	6,6,6	0.37	0
2	SO4	B	709	-	4,4,4	0.18	0	6,6,6	0.33	0
3	T5A	A	501[A]	-	48,59,59	1.36	5 (10%)	59,93,93	2.07	15 (25%)
2	SO4	A	704	-	4,4,4	0.12	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	706	-	4,4,4	0.11	0	6,6,6	0.32	0
2	SO4	B	711	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	B	712	-	4,4,4	0.13	0	6,6,6	0.37	0
2	SO4	A	701	-	4,4,4	0.17	0	6,6,6	0.22	0
2	SO4	B	705	-	4,4,4	0.18	0	6,6,6	0.49	0
2	SO4	D	716	-	4,4,4	0.16	0	6,6,6	0.33	0
3	T5A	D	504[B]	-	48,59,59	1.32	7 (14%)	59,93,93	2.04	14 (23%)
3	T5A	C	503[B]	-	48,59,59	1.28	4 (8%)	59,93,93	1.99	13 (22%)
2	SO4	D	713	-	4,4,4	0.25	0	6,6,6	0.28	0
3	T5A	B	502[A]	-	48,59,59	1.29	9 (18%)	59,93,93	2.04	16 (27%)
2	SO4	B	707	-	4,4,4	0.20	0	6,6,6	0.31	0
3	T5A	A	501[B]	-	48,59,59	1.36	5 (10%)	59,93,93	2.03	15 (25%)
2	SO4	C	714	-	4,4,4	0.18	0	6,6,6	0.13	0
2	SO4	C	715	-	4,4,4	0.16	0	6,6,6	0.27	0
2	SO4	A	703	-	4,4,4	0.21	0	6,6,6	0.28	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	T5A	D	504[B]	-	-	8/40/72/72	0/5/5/5
3	T5A	A	501[B]	-	-	6/40/72/72	0/5/5/5
3	T5A	A	501[A]	-	-	7/40/72/72	0/5/5/5
3	T5A	C	503[A]	-	-	11/40/72/72	0/5/5/5
3	T5A	C	503[B]	-	-	4/40/72/72	0/5/5/5
3	T5A	D	504[A]	-	-	11/40/72/72	0/5/5/5
3	T5A	B	502[A]	-	-	6/40/72/72	0/5/5/5
3	T5A	B	502[B]	-	-	10/40/72/72	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501[A]	T5A	O4B-C4B	5.01	1.33	1.23
3	A	501[B]	T5A	O4B-C4B	5.01	1.33	1.23
3	C	503[A]	T5A	O4B-C4B	4.61	1.32	1.23
3	C	503[B]	T5A	O4B-C4B	4.61	1.32	1.23
3	B	502[A]	T5A	O4B-C4B	4.44	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[B]	T5A	O4B-C4B	4.44	1.32	1.23
3	D	504[A]	T5A	O4B-C4B	4.37	1.31	1.23
3	D	504[B]	T5A	O4B-C4B	4.37	1.31	1.23
3	A	501[A]	T5A	C4B-C5B	3.16	1.50	1.44
3	A	501[B]	T5A	C4B-C5B	3.16	1.50	1.44
3	D	504[A]	T5A	O4F-C1F	3.06	1.45	1.41
3	D	504[B]	T5A	O4F-C1F	3.06	1.45	1.41
3	A	501[A]	T5A	C6B-C5B	3.02	1.39	1.34
3	A	501[B]	T5A	C6B-C5B	3.02	1.39	1.34
3	C	503[A]	T5A	C6B-C5B	2.98	1.39	1.34
3	C	503[B]	T5A	C6B-C5B	2.98	1.39	1.34
3	C	503[A]	T5A	O4F-C1F	2.88	1.45	1.41
3	C	503[B]	T5A	O4F-C1F	2.88	1.45	1.41
3	D	504[A]	T5A	C6B-C5B	2.79	1.39	1.34
3	D	504[B]	T5A	C6B-C5B	2.79	1.39	1.34
3	B	502[A]	T5A	O4F-C1F	2.64	1.44	1.41
3	B	502[B]	T5A	O4F-C1F	2.64	1.44	1.41
3	B	502[A]	T5A	C6B-C5B	2.64	1.38	1.34
3	B	502[B]	T5A	C6B-C5B	2.64	1.38	1.34
3	A	501[A]	T5A	C2B-N1B	2.56	1.42	1.38
3	A	501[B]	T5A	C2B-N1B	2.56	1.42	1.38
3	B	502[A]	T5A	C2B-N1B	2.38	1.42	1.38
3	B	502[B]	T5A	C2B-N1B	2.38	1.42	1.38
3	C	503[A]	T5A	C2A-N3A	2.37	1.35	1.32
3	C	503[B]	T5A	C2A-N3A	2.37	1.35	1.32
3	B	502[A]	T5A	C2A-N3A	2.33	1.35	1.32
3	B	502[B]	T5A	C2A-N3A	2.33	1.35	1.32
3	B	502[A]	T5A	C4B-N3B	-2.26	1.34	1.38
3	B	502[B]	T5A	C4B-N3B	-2.26	1.34	1.38
3	D	504[A]	T5A	C2A-N3A	2.24	1.35	1.32
3	D	504[B]	T5A	C2A-N3A	2.24	1.35	1.32
3	D	504[A]	T5A	C4B-N3B	-2.21	1.34	1.38
3	D	504[B]	T5A	C4B-N3B	-2.21	1.34	1.38
3	A	501[A]	T5A	C5A-C4A	-2.20	1.35	1.40
3	A	501[B]	T5A	C5A-C4A	-2.20	1.35	1.40
3	D	504[A]	T5A	C5A-C4A	-2.17	1.35	1.40
3	D	504[B]	T5A	C5A-C4A	-2.17	1.35	1.40
3	D	504[A]	T5A	C4B-C5B	2.09	1.48	1.44
3	D	504[B]	T5A	C4B-C5B	2.09	1.48	1.44
3	B	502[A]	T5A	C5A-C4A	-2.09	1.35	1.40
3	B	502[B]	T5A	C5A-C4A	-2.09	1.35	1.40
3	B	502[A]	T5A	C4B-C5B	2.06	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[B]	T5A	C4B-C5B	2.06	1.48	1.44
3	B	502[A]	T5A	C8A-N7A	2.04	1.38	1.34
3	B	502[B]	T5A	C8A-N7A	2.04	1.38	1.34

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	504[A]	T5A	C5B-C4B-N3B	6.30	120.69	115.31
3	D	504[B]	T5A	C5B-C4B-N3B	6.30	120.69	115.31
3	B	502[A]	T5A	C5B-C4B-N3B	5.81	120.27	115.31
3	B	502[B]	T5A	C5B-C4B-N3B	5.81	120.27	115.31
3	D	504[A]	T5A	C4B-N3B-C2B	-5.76	119.89	127.35
3	D	504[B]	T5A	C4B-N3B-C2B	-5.76	119.89	127.35
3	C	503[A]	T5A	O4B-C4B-C5B	-5.62	118.39	124.90
3	C	503[B]	T5A	O4B-C4B-C5B	-5.62	118.39	124.90
3	D	504[A]	T5A	N3A-C2A-N1A	-5.54	120.02	128.68
3	D	504[B]	T5A	N3A-C2A-N1A	-5.54	120.02	128.68
3	B	502[A]	T5A	C4B-N3B-C2B	-5.49	120.24	127.35
3	B	502[B]	T5A	C4B-N3B-C2B	-5.49	120.24	127.35
3	C	503[A]	T5A	C4B-N3B-C2B	-5.24	120.57	127.35
3	C	503[B]	T5A	C4B-N3B-C2B	-5.24	120.57	127.35
3	A	501[A]	T5A	C4B-N3B-C2B	-5.17	120.66	127.35
3	A	501[B]	T5A	C4B-N3B-C2B	-5.17	120.66	127.35
3	A	501[A]	T5A	C1F-N9A-C4A	-5.16	117.58	126.64
3	A	501[B]	T5A	C1F-N9A-C4A	-5.16	117.58	126.64
3	C	503[A]	T5A	C5B-C4B-N3B	5.11	119.67	115.31
3	C	503[B]	T5A	C5B-C4B-N3B	5.11	119.67	115.31
3	A	501[A]	T5A	N3A-C2A-N1A	-4.72	121.30	128.68
3	A	501[B]	T5A	N3A-C2A-N1A	-4.72	121.30	128.68
3	A	501[A]	T5A	N3B-C2B-N1B	4.69	121.11	114.89
3	A	501[B]	T5A	N3B-C2B-N1B	4.69	121.11	114.89
3	C	503[A]	T5A	N3A-C2A-N1A	-4.52	121.61	128.68
3	C	503[B]	T5A	N3A-C2A-N1A	-4.52	121.61	128.68
3	B	502[A]	T5A	N3B-C2B-N1B	4.52	120.89	114.89
3	B	502[B]	T5A	N3B-C2B-N1B	4.52	120.89	114.89
3	B	502[A]	T5A	N3A-C2A-N1A	-4.42	121.77	128.68
3	B	502[B]	T5A	N3A-C2A-N1A	-4.42	121.77	128.68
3	D	504[A]	T5A	N3B-C2B-N1B	4.40	120.73	114.89
3	D	504[B]	T5A	N3B-C2B-N1B	4.40	120.73	114.89
3	A	501[A]	T5A	C5B-C4B-N3B	4.36	119.03	115.31
3	A	501[B]	T5A	C5B-C4B-N3B	4.36	119.03	115.31
3	B	502[B]	T5A	PC-O3B-PB	-4.29	118.12	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502[A]	T5A	PD-O3C-PC	-4.29	118.12	132.83
3	C	503[A]	T5A	C1F-N9A-C4A	-4.14	119.36	126.64
3	C	503[B]	T5A	C1F-N9A-C4A	-4.14	119.36	126.64
3	C	503[A]	T5A	PD-O3C-PC	-4.09	118.78	132.83
3	A	501[A]	T5A	C7B-C5B-C4B	4.08	123.26	118.77
3	A	501[B]	T5A	C7B-C5B-C4B	4.08	123.26	118.77
3	C	503[A]	T5A	N3B-C2B-N1B	4.06	120.29	114.89
3	C	503[B]	T5A	N3B-C2B-N1B	4.06	120.29	114.89
3	C	503[B]	T5A	PC-O3B-PB	-4.01	119.05	132.83
3	D	504[A]	T5A	PD-O3C-PC	-3.96	119.25	132.83
3	D	504[A]	T5A	O4B-C4B-C5B	-3.91	120.37	124.90
3	D	504[B]	T5A	O4B-C4B-C5B	-3.91	120.37	124.90
3	A	501[A]	T5A	PD-O3C-PC	-3.82	119.73	132.83
3	D	504[B]	T5A	PC-O3B-PB	-3.56	120.61	132.83
3	B	502[B]	T5A	PB-O3A-PA	-3.49	120.84	132.83
3	A	501[A]	T5A	O3F-C3F-C2F	-3.46	100.63	111.82
3	A	501[B]	T5A	O3F-C3F-C2F	-3.46	100.63	111.82
3	D	504[A]	T5A	C5B-C6B-N1B	-3.45	119.79	123.34
3	D	504[B]	T5A	C5B-C6B-N1B	-3.45	119.79	123.34
3	A	501[A]	T5A	C7B-C5B-C6B	-3.38	118.33	122.85
3	A	501[B]	T5A	C7B-C5B-C6B	-3.38	118.33	122.85
3	A	501[A]	T5A	C5B-C6B-N1B	-3.31	119.94	123.34
3	A	501[B]	T5A	C5B-C6B-N1B	-3.31	119.94	123.34
3	B	502[A]	T5A	O4B-C4B-C5B	-3.27	121.11	124.90
3	B	502[B]	T5A	O4B-C4B-C5B	-3.27	121.11	124.90
3	D	504[B]	T5A	PE-O3D-PD	-3.24	121.72	132.83
3	B	502[A]	T5A	C5B-C6B-N1B	-3.23	120.02	123.34
3	B	502[B]	T5A	C5B-C6B-N1B	-3.23	120.02	123.34
3	D	504[A]	T5A	C1F-N9A-C4A	-3.17	121.08	126.64
3	D	504[B]	T5A	C1F-N9A-C4A	-3.17	121.08	126.64
3	B	502[A]	T5A	C3F-C2F-C1F	3.11	105.67	100.98
3	B	502[B]	T5A	C3F-C2F-C1F	3.11	105.67	100.98
3	D	504[A]	T5A	C3F-C2F-C1F	3.01	105.50	100.98
3	D	504[B]	T5A	C3F-C2F-C1F	3.01	105.50	100.98
3	C	503[B]	T5A	PD-O3C-PC	-2.97	122.63	132.83
3	C	503[A]	T5A	C3F-C2F-C1F	2.95	105.43	100.98
3	C	503[B]	T5A	C3F-C2F-C1F	2.95	105.43	100.98
3	B	502[B]	T5A	PD-O3C-PC	-2.91	122.84	132.83
3	B	502[A]	T5A	C1F-N9A-C4A	-2.90	121.54	126.64
3	B	502[B]	T5A	C1F-N9A-C4A	-2.90	121.54	126.64
3	A	501[B]	T5A	PC-O3B-PB	-2.89	122.89	132.83
3	B	502[B]	T5A	PE-O3D-PD	-2.82	123.16	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502[A]	T5A	PE-O3D-PD	-2.77	123.33	132.83
3	D	504[A]	T5A	O2B-C2B-N1B	-2.75	119.13	122.79
3	D	504[B]	T5A	O2B-C2B-N1B	-2.75	119.13	122.79
3	C	503[B]	T5A	PE-O3D-PD	-2.72	123.49	132.83
3	D	504[A]	T5A	PE-O3D-PD	-2.72	123.50	132.83
3	C	503[A]	T5A	O2B-C2B-N1B	-2.65	119.26	122.79
3	C	503[B]	T5A	O2B-C2B-N1B	-2.65	119.26	122.79
3	A	501[A]	T5A	C2F-C3F-C4F	2.64	107.77	102.64
3	A	501[B]	T5A	C2F-C3F-C4F	2.64	107.77	102.64
3	A	501[A]	T5A	PC-O3B-PB	-2.61	123.85	132.83
3	C	503[B]	T5A	PB-O3A-PA	-2.48	124.31	132.83
3	B	502[A]	T5A	N6A-C6A-N1A	2.42	123.60	118.57
3	B	502[B]	T5A	N6A-C6A-N1A	2.42	123.60	118.57
3	A	501[B]	T5A	PB-O3A-PA	-2.42	124.52	132.83
3	A	501[B]	T5A	PD-O3C-PC	-2.42	124.53	132.83
3	B	502[A]	T5A	C7B-C5B-C4B	2.39	121.39	118.77
3	B	502[B]	T5A	C7B-C5B-C4B	2.39	121.39	118.77
3	D	504[A]	T5A	C7B-C5B-C4B	2.37	121.38	118.77
3	D	504[B]	T5A	C7B-C5B-C4B	2.37	121.38	118.77
3	A	501[A]	T5A	O5F-C5F-C4F	2.35	117.07	108.99
3	C	503[A]	T5A	O5F-C5F-C4F	2.34	117.03	108.99
3	C	503[A]	T5A	O4F-C4F-C5F	2.31	116.98	109.37
3	A	501[B]	T5A	PE-O3D-PD	-2.26	125.09	132.83
3	B	502[A]	T5A	O4E-C1E-N1B	2.21	111.82	107.86
3	B	502[B]	T5A	O4E-C1E-N1B	2.21	111.82	107.86
3	B	502[A]	T5A	PC-O3B-PB	-2.21	125.25	132.83
3	A	501[A]	T5A	O2B-C2B-N1B	-2.20	119.87	122.79
3	A	501[B]	T5A	O2B-C2B-N1B	-2.20	119.87	122.79
3	B	502[A]	T5A	C5A-C6A-N6A	-2.16	117.07	120.35
3	B	502[B]	T5A	C5A-C6A-N6A	-2.16	117.07	120.35
3	D	504[B]	T5A	O5F-C5F-C4F	2.11	116.27	108.99
3	B	502[A]	T5A	O5F-C5F-C4F	2.11	116.24	108.99
3	D	504[A]	T5A	C2E-C3E-C4E	2.09	107.12	102.76
3	D	504[B]	T5A	C2E-C3E-C4E	2.09	107.12	102.76
3	C	503[A]	T5A	C5B-C6B-N1B	-2.09	121.18	123.34
3	C	503[B]	T5A	C5B-C6B-N1B	-2.09	121.18	123.34
3	A	501[A]	T5A	PE-O3D-PD	-2.04	125.81	132.83

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501[A]	T5A	PB-O3A-PA-O5E
3	A	501[A]	T5A	C5F-O5F-PE-O1E
3	A	501[B]	T5A	C5F-O5F-PE-O3D
3	B	502[A]	T5A	O4E-C4E-C5E-O5E
3	B	502[A]	T5A	C3E-C4E-C5E-O5E
3	B	502[B]	T5A	C5E-O5E-PA-O1A
3	B	502[B]	T5A	C5E-O5E-PA-O2A
3	B	502[B]	T5A	C5E-O5E-PA-O3A
3	B	502[B]	T5A	C5F-O5F-PE-O3D
3	B	502[B]	T5A	C5F-O5F-PE-O1E
3	C	503[A]	T5A	O4E-C4E-C5E-O5E
3	C	503[A]	T5A	C3E-C4E-C5E-O5E
3	C	503[A]	T5A	C5E-O5E-PA-O3A
3	C	503[A]	T5A	C5F-O5F-PE-O1E
3	C	503[B]	T5A	C5F-O5F-PE-O2E
3	D	504[A]	T5A	O4E-C4E-C5E-O5E
3	D	504[A]	T5A	C3E-C4E-C5E-O5E
3	D	504[A]	T5A	C5E-O5E-PA-O2A
3	D	504[A]	T5A	C5F-O5F-PE-O1E
3	D	504[B]	T5A	C5F-O5F-PE-O3D
3	D	504[B]	T5A	C5F-O5F-PE-O1E
3	D	504[B]	T5A	C5F-O5F-PE-O2E
3	A	501[B]	T5A	O4F-C4F-C5F-O5F
3	A	501[B]	T5A	C3F-C4F-C5F-O5F
3	C	503[A]	T5A	O4F-C4F-C5F-O5F
3	C	503[A]	T5A	C3F-C4F-C5F-O5F
3	B	502[B]	T5A	PE-O3D-PD-O2D
3	C	503[B]	T5A	PE-O3D-PD-O2D
3	D	504[B]	T5A	PC-O3C-PD-O2D
3	D	504[B]	T5A	C4F-C5F-O5F-PE
3	D	504[A]	T5A	PD-O3D-PE-O5F
3	A	501[A]	T5A	C5F-O5F-PE-O3D
3	C	503[A]	T5A	C5F-O5F-PE-O3D
3	C	503[B]	T5A	C5F-O5F-PE-O3D
3	D	504[A]	T5A	C5F-O5F-PE-O3D
3	D	504[A]	T5A	PB-O3B-PC-O1C
3	B	502[A]	T5A	C4F-C5F-O5F-PE
3	A	501[B]	T5A	C5F-O5F-PE-O1E
3	A	501[B]	T5A	C5F-O5F-PE-O2E
3	B	502[B]	T5A	C5F-O5F-PE-O2E
3	C	503[A]	T5A	C5E-O5E-PA-O1A
3	C	503[A]	T5A	C5E-O5E-PA-O2A
3	C	503[A]	T5A	C5F-O5F-PE-O2E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	504[A]	T5A	C5F-O5F-PE-O2E
3	D	504[A]	T5A	C4F-C5F-O5F-PE
3	B	502[B]	T5A	PE-O3D-PD-O1D
3	B	502[B]	T5A	C4F-C5F-O5F-PE
3	A	501[A]	T5A	C3F-C4F-C5F-O5F
3	A	501[B]	T5A	PD-O3D-PE-O2E
3	C	503[A]	T5A	C4F-C5F-O5F-PE
3	D	504[B]	T5A	O4F-C4F-C5F-O5F
3	B	502[A]	T5A	C5F-O5F-PE-O3D
3	A	501[A]	T5A	O4F-C4F-C5F-O5F
3	A	501[A]	T5A	PD-O3C-PC-O2C
3	C	503[B]	T5A	PE-O3D-PD-O1D
3	D	504[A]	T5A	PB-O3B-PC-O2C
3	D	504[A]	T5A	PD-O3C-PC-O2C
3	D	504[B]	T5A	PC-O3C-PD-O1D
3	A	501[A]	T5A	C5F-O5F-PE-O2E
3	B	502[A]	T5A	C5E-O5E-PA-O2A
3	B	502[A]	T5A	C5F-O5F-PE-O2E
3	B	502[B]	T5A	C3F-C4F-C5F-O5F
3	D	504[B]	T5A	C3F-C4F-C5F-O5F

There are no ring outliers.

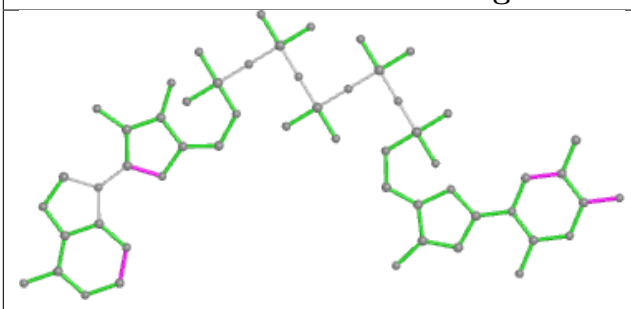
11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503[A]	T5A	3	0
3	D	504[A]	T5A	2	0
2	A	708	SO4	1	0
3	B	502[B]	T5A	4	0
3	A	501[A]	T5A	3	0
3	D	504[B]	T5A	4	0
3	C	503[B]	T5A	2	0
2	D	713	SO4	1	0
3	B	502[A]	T5A	3	0
3	A	501[B]	T5A	2	0
2	C	715	SO4	1	0

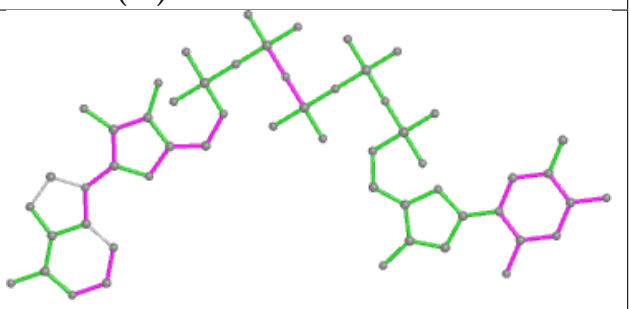
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

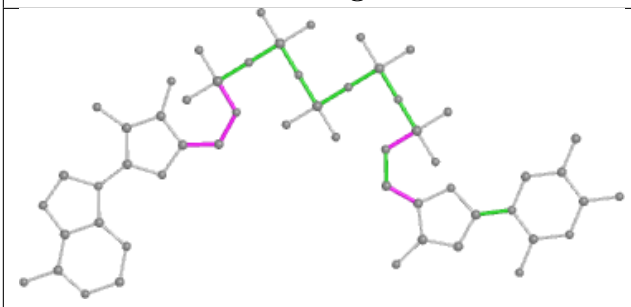
Ligand T5A C 503 (A)



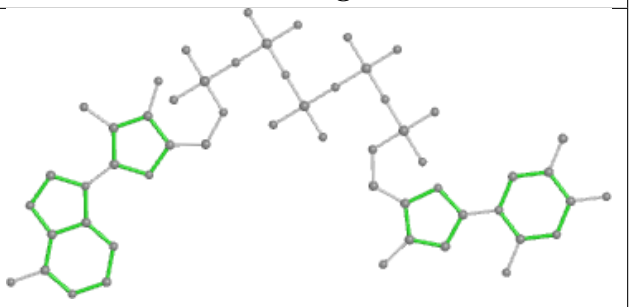
Bond lengths



Bond angles

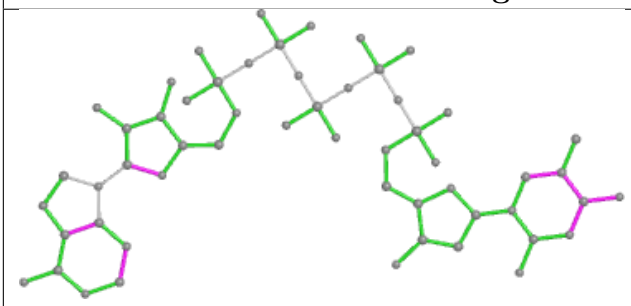


Torsions

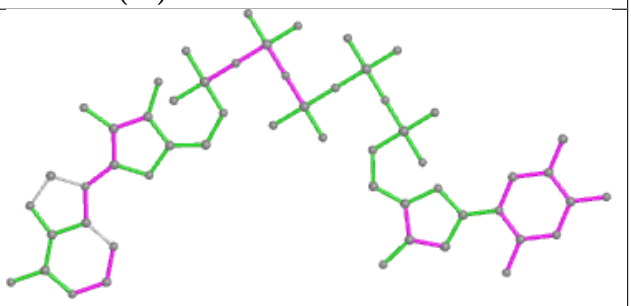


Rings

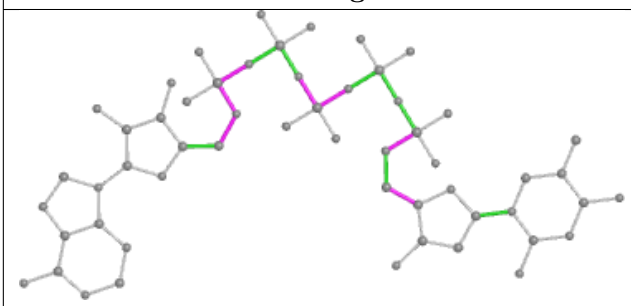
Ligand T5A D 504 (A)



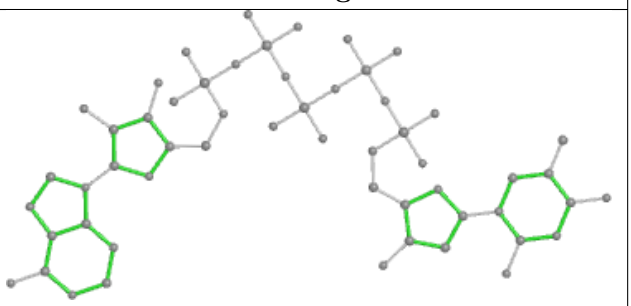
Bond lengths



Bond angles

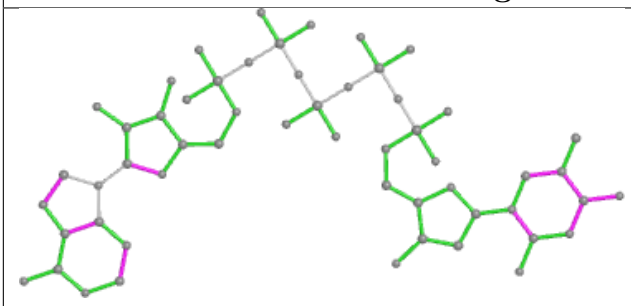


Torsions

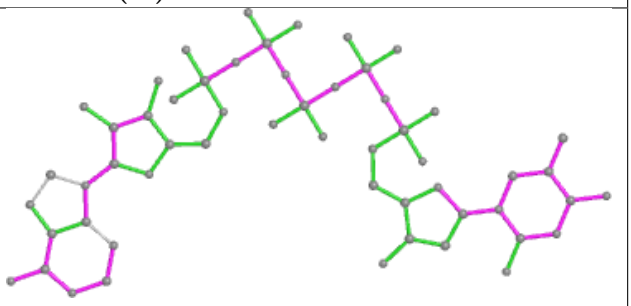


Rings

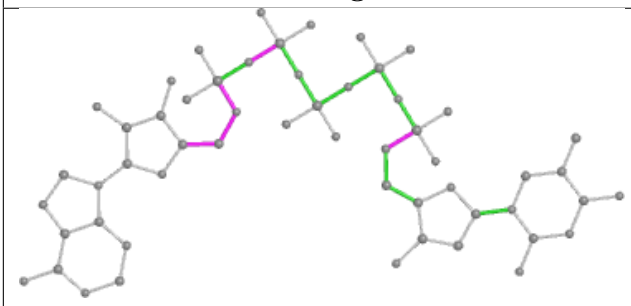
Ligand T5A B 502 (B)



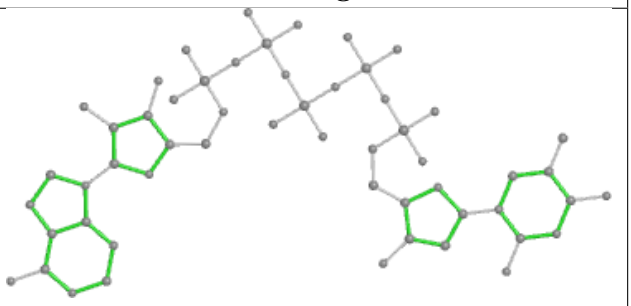
Bond lengths



Bond angles

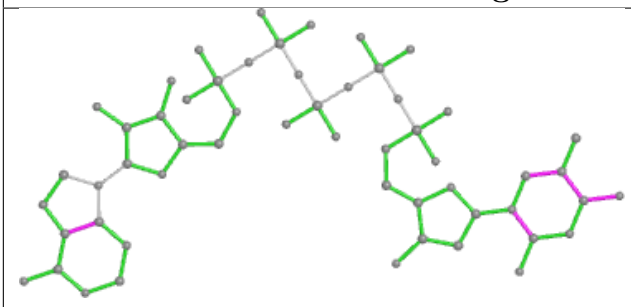


Torsions

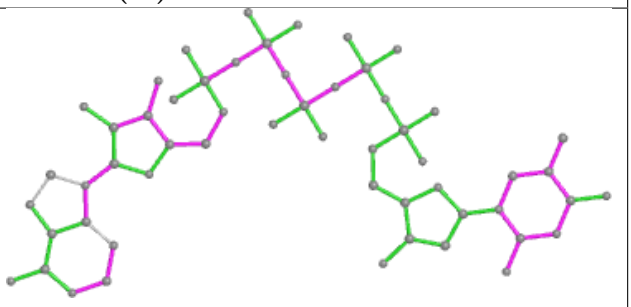


Rings

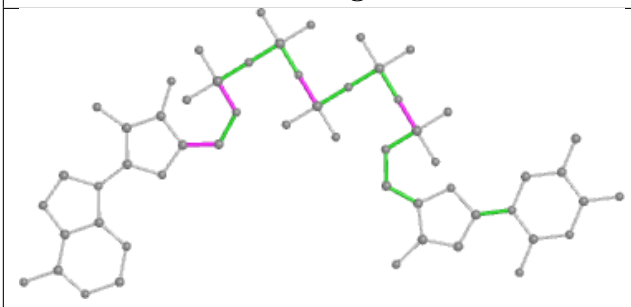
Ligand T5A A 501 (A)



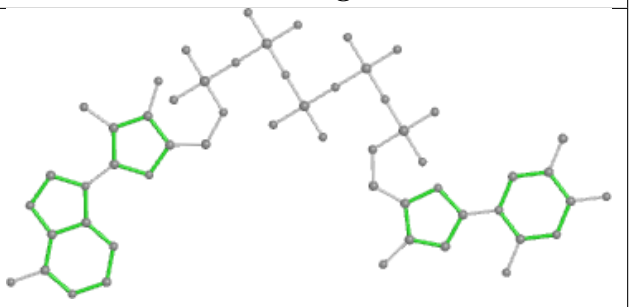
Bond lengths



Bond angles

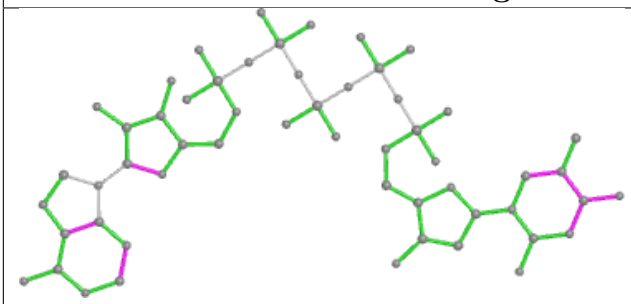


Torsions

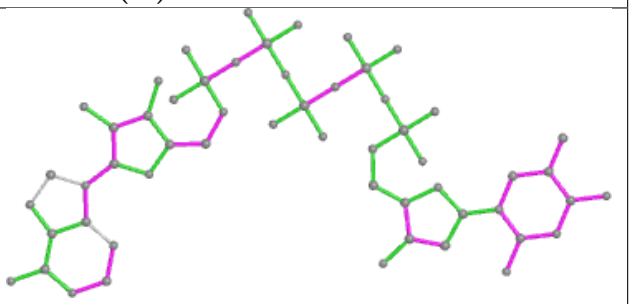


Rings

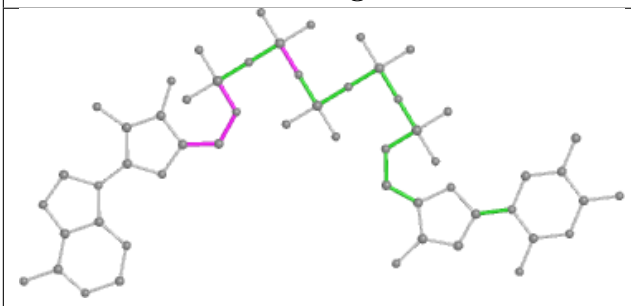
Ligand T5A D 504 (B)



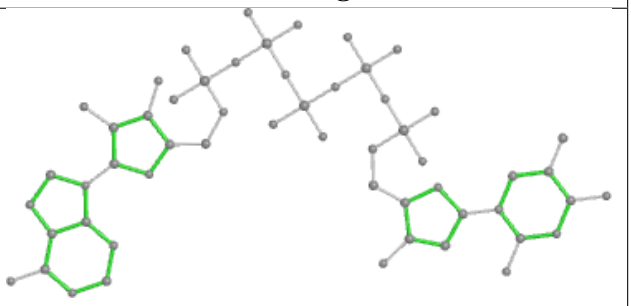
Bond lengths



Bond angles

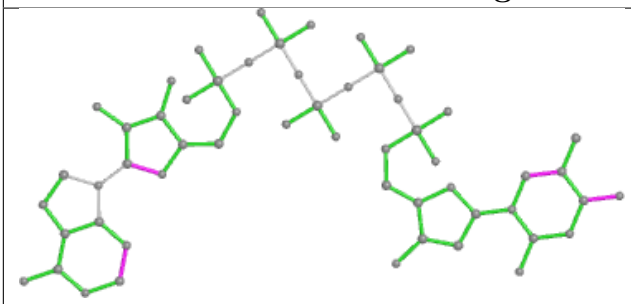


Torsions

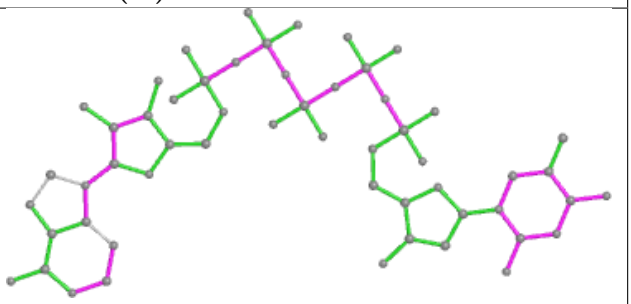


Rings

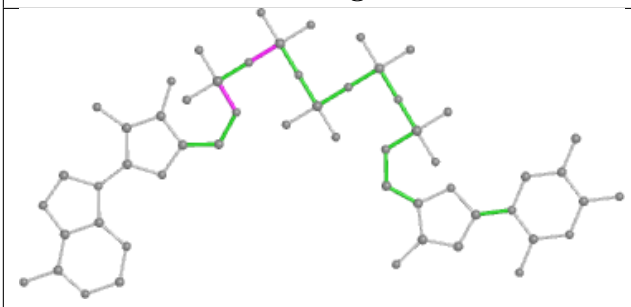
Ligand T5A C 503 (B)



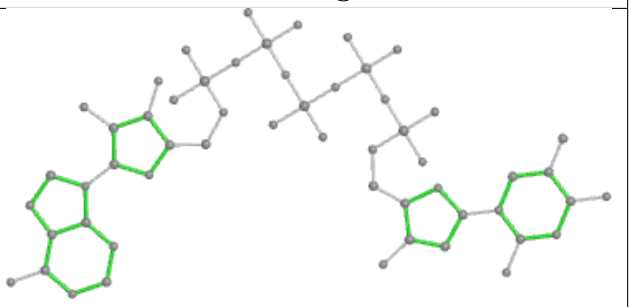
Bond lengths



Bond angles

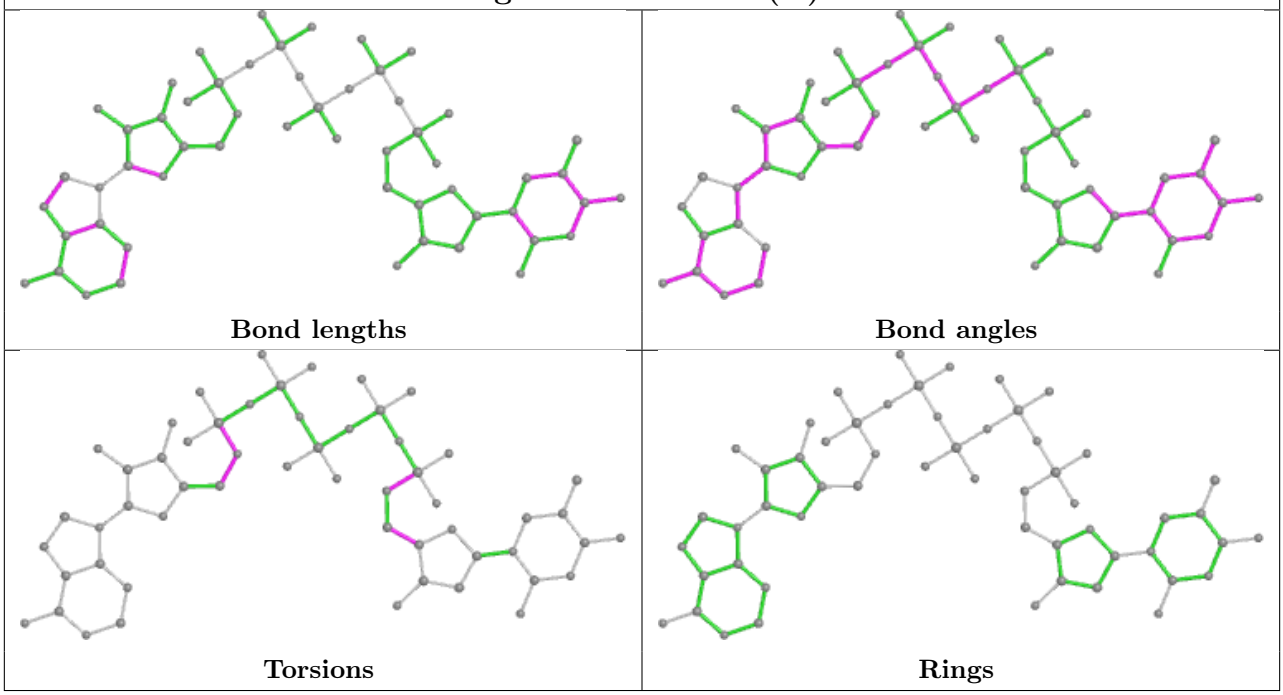


Torsions

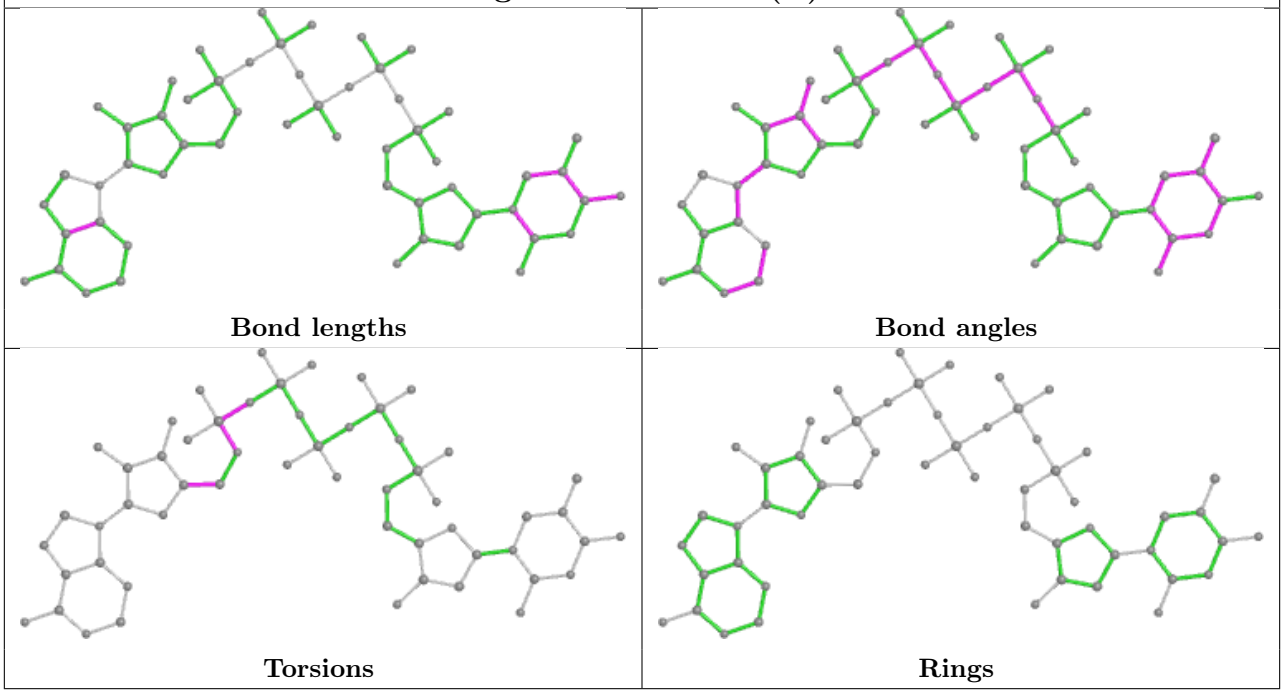


Rings

Ligand T5A B 502 (A)



Ligand T5A A 501 (B)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	331/334 (99%)	-0.34	8 (2%)	59	30	13, 27, 45, 55	0
1	B	333/334 (99%)	-0.36	3 (0%)	84	62	14, 27, 45, 52	0
1	C	330/334 (98%)	-0.39	3 (0%)	84	62	16, 27, 40, 54	0
1	D	328/334 (98%)	-0.28	9 (2%)	54	26	16, 30, 44, 59	0
All	All	1322/1336 (98%)	-0.35	23 (1%)	70	41	13, 28, 44, 59	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	20	SER	4.5
1	D	50	SER	4.0
1	A	200	GLY	4.0
1	D	49	ALA	3.8
1	C	201	GLU	3.6
1	D	200	GLY	3.1
1	B	85	GLN	2.5
1	A	87	GLY	2.5
1	D	51	GLY	2.5
1	D	53	SER	2.5
1	A	21	HIS	2.5
1	A	197	ALA	2.3
1	D	201	GLU	2.3
1	A	352	VAL	2.1
1	C	351	GLY	2.1
1	C	279	ASP	2.1
1	A	201	GLU	2.1
1	D	279	ASP	2.1
1	A	50	SER	2.1
1	B	197	ALA	2.1
1	B	352	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	22	MET	2.0
1	A	202	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	704	5/5	0.88	0.29	68,68,69,69	0
2	SO4	C	714	5/5	0.88	0.45	66,66,66,66	0
2	SO4	A	701	5/5	0.89	0.34	59,60,60,60	0
2	SO4	B	710	5/5	0.91	0.35	51,51,51,51	0
3	T5A	D	504[A]	55/55	0.91	0.19	29,40,48,49	23
3	T5A	D	504[B]	55/55	0.91	0.19	29,41,48,49	23
3	T5A	A	501[A]	55/55	0.92	0.18	27,32,33,33	23
3	T5A	A	501[B]	55/55	0.92	0.18	27,32,33,33	23
3	T5A	B	502[A]	55/55	0.92	0.22	26,32,33,34	23
3	T5A	B	502[B]	55/55	0.92	0.22	26,32,33,34	23
3	T5A	C	503[A]	55/55	0.92	0.22	26,32,33,33	23
3	T5A	C	503[B]	55/55	0.92	0.22	26,32,33,33	23
2	SO4	B	711	5/5	0.92	0.28	69,69,69,69	0
2	SO4	B	709	5/5	0.92	0.34	54,54,55,55	0
2	SO4	A	703	5/5	0.93	0.26	55,55,56,56	0
2	SO4	B	707	5/5	0.93	0.26	54,54,55,55	0
2	SO4	B	706	5/5	0.94	0.15	47,47,47,47	0
2	SO4	D	716	5/5	0.95	0.24	61,61,61,61	0
2	SO4	B	712	5/5	0.95	0.32	60,60,61,61	0
2	SO4	D	713	5/5	0.95	0.18	37,37,37,38	0
2	SO4	B	705	5/5	0.96	0.25	31,33,33,34	0

Continued on next page...

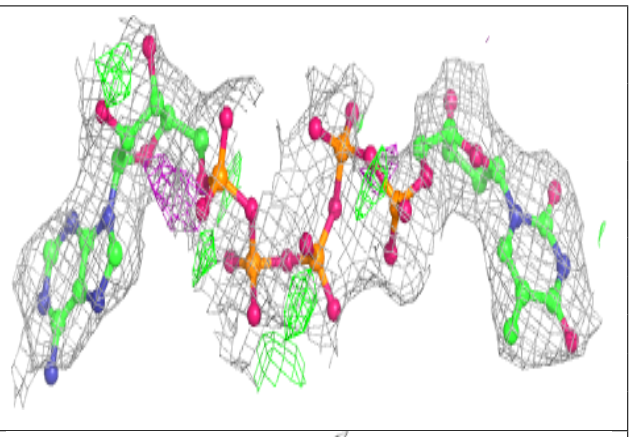
Continued from previous page...

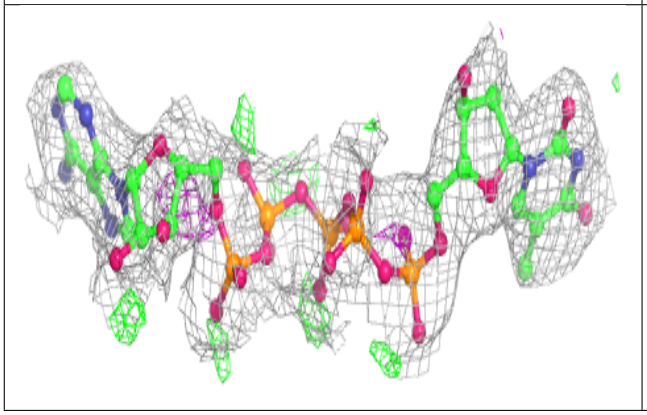
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	708	5/5	0.98	0.13	43,44,45,45	0
2	SO4	C	715	5/5	0.98	0.12	32,32,32,32	0
2	SO4	A	702	5/5	0.98	0.15	28,28,29,29	0

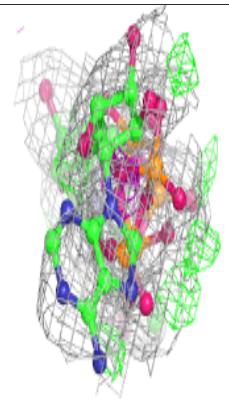
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T5A D 504 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

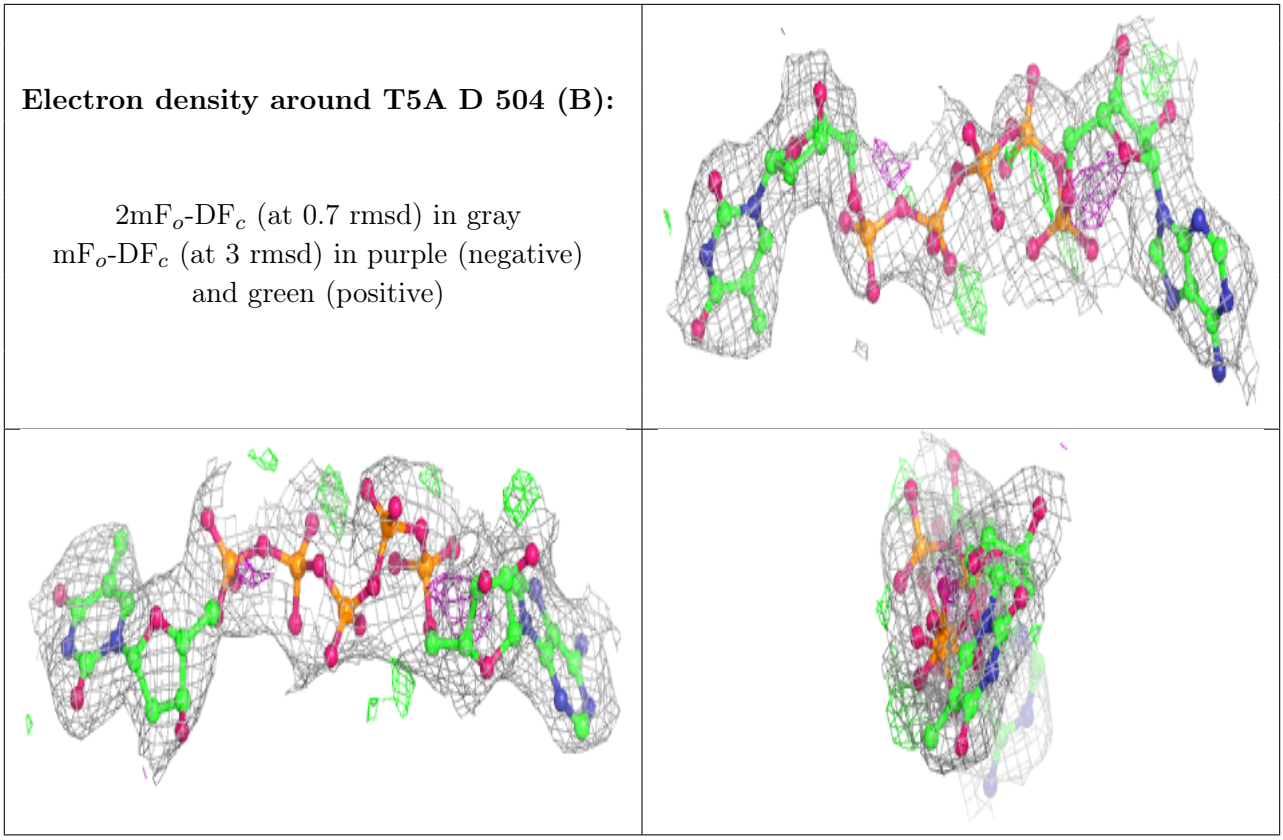






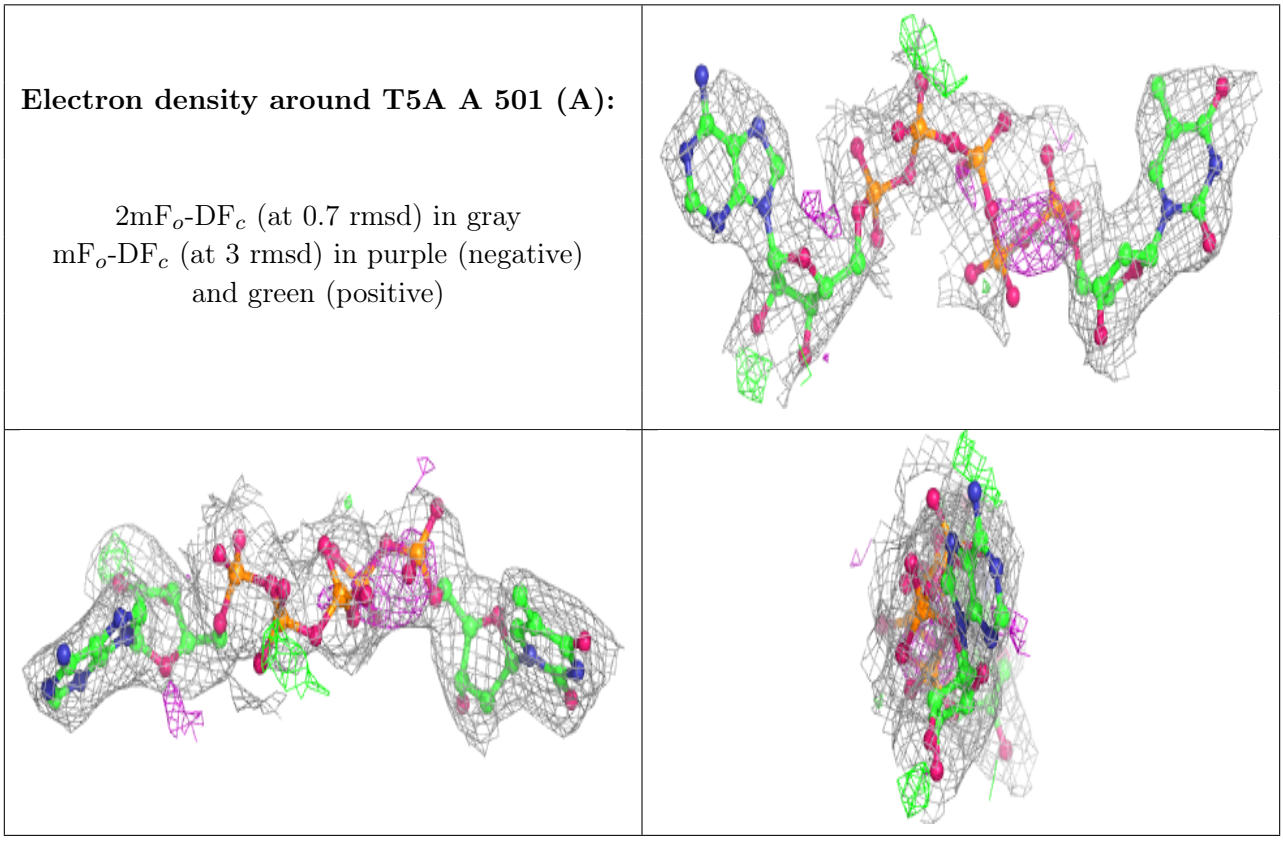
Electron density around T5A D 504 (B):

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



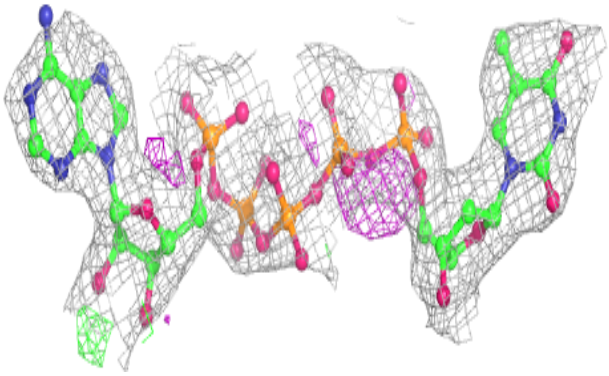
Electron density around T5A A 501 (A):

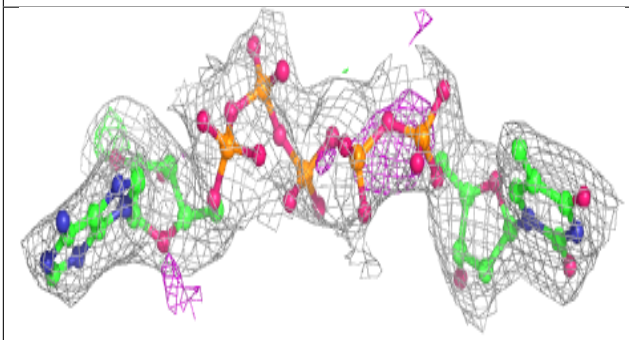
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

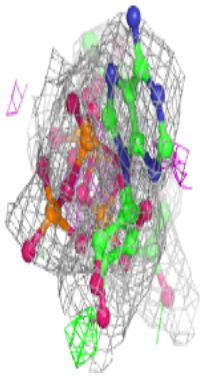


Electron density around T5A A 501 (B):

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

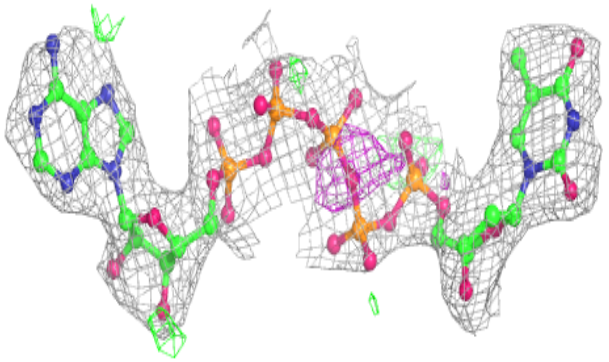


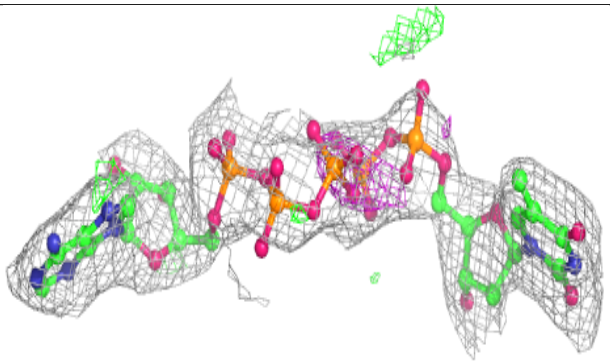


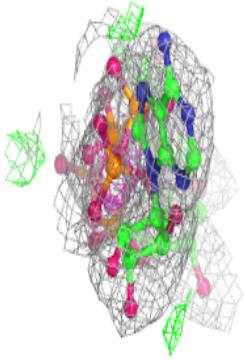


Electron density around T5A B 502 (A):

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

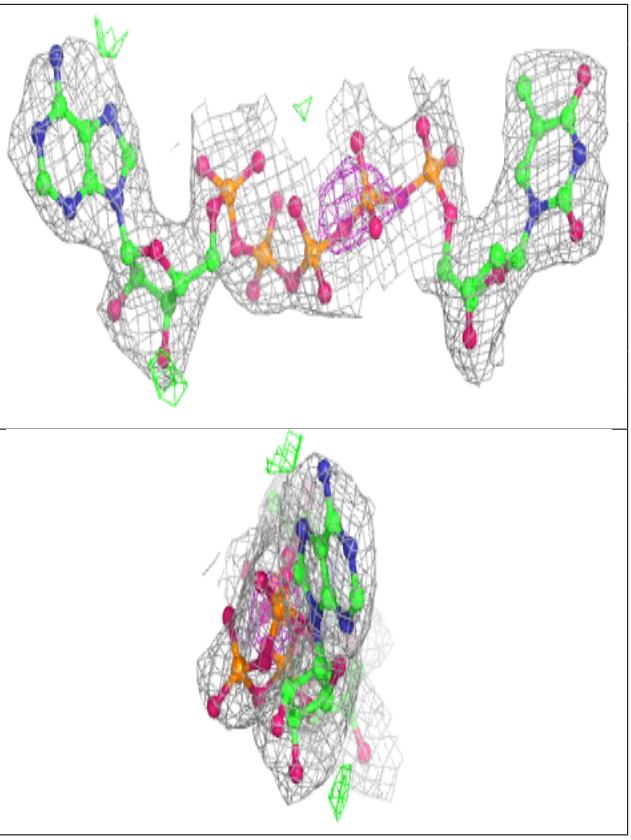






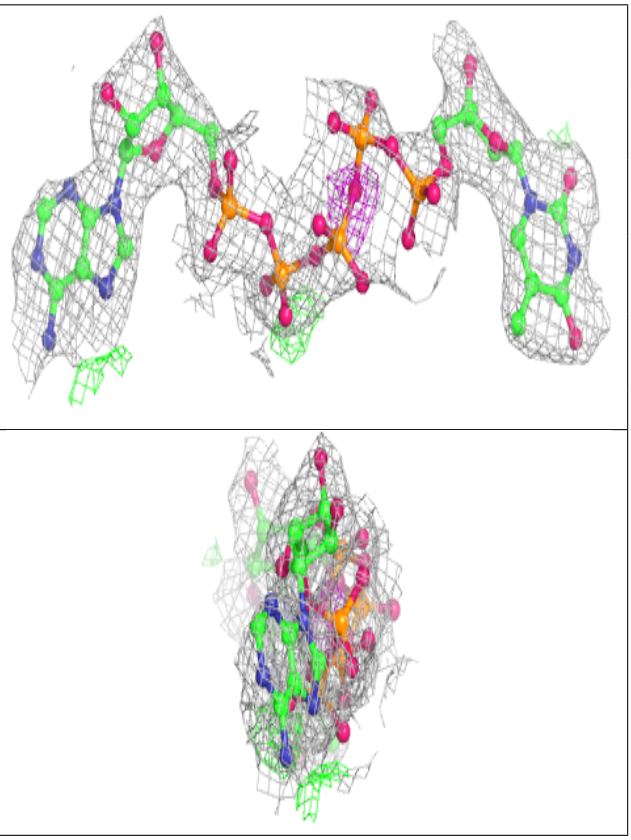
Electron density around T5A B 502 (B):

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



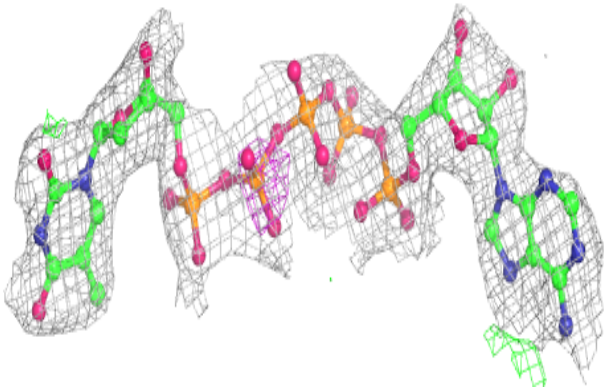
Electron density around T5A C 503 (A):

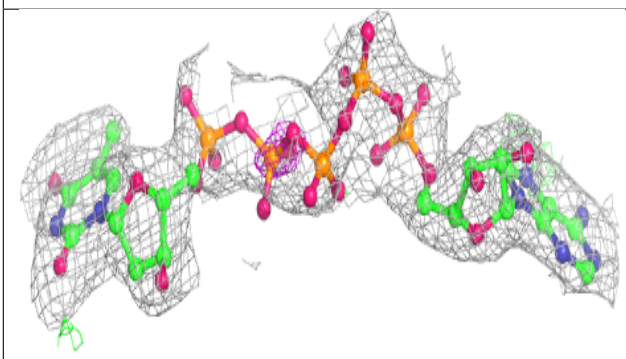
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

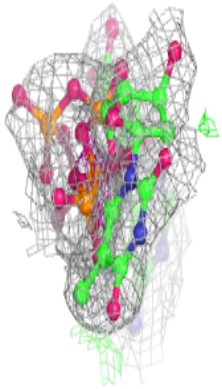


Electron density around T5A C 503 (B):

$2mF_o$-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.