Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 01:44 AM EDT

PDB ID	:	4G8L
Title	:	Active state of intact sensor domain of human RNase L with 2-5A bound
Authors	:	Han, Y.; Whitney, G.; Donovan, J.; Korennykh, A.
Deposited on	:	2012-07-23
Resolution	:	2.80 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:

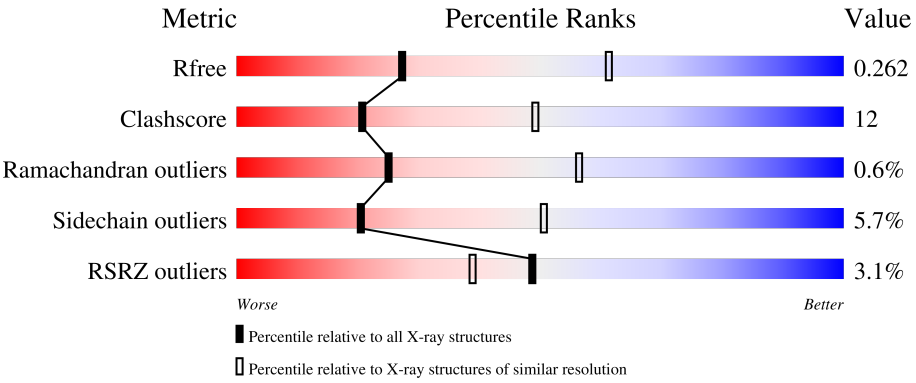
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	337	3% 68% 20% • 9%
1	B	337	3% 66% 19% • 13%
1	C	337	2% 67% 20% • 11%
1	D	337	2% 66% 19% • 13%

2 Entry composition (i)

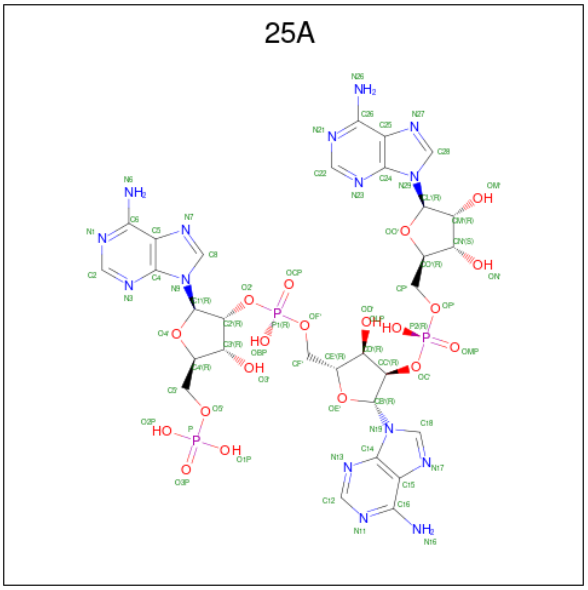
There are 2 unique types of molecules in this entry. The entry contains 9415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-5A-dependent ribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2359	1475	427	447	10			
1	B	294	Total	C	N	O	S	0	0	0
			2249	1413	403	424	9			
1	C	300	Total	C	N	O	S	0	0	0
			2294	1438	413	434	9			
1	D	294	Total	C	N	O	S	0	0	0
			2245	1411	400	425	9			

- Molecule 2 is 5'-O-MONOPHOSPHORYLADENYLYL(2'->5')ADENYLYL(2'->5')ADENOSINE (three-letter code: 25A) (formula: $C_{30}H_{38}N_{15}O_{19}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			67	30	15	19	3		
2	B	1	Total	C	N	O	P	0	0
			67	30	15	19	3		

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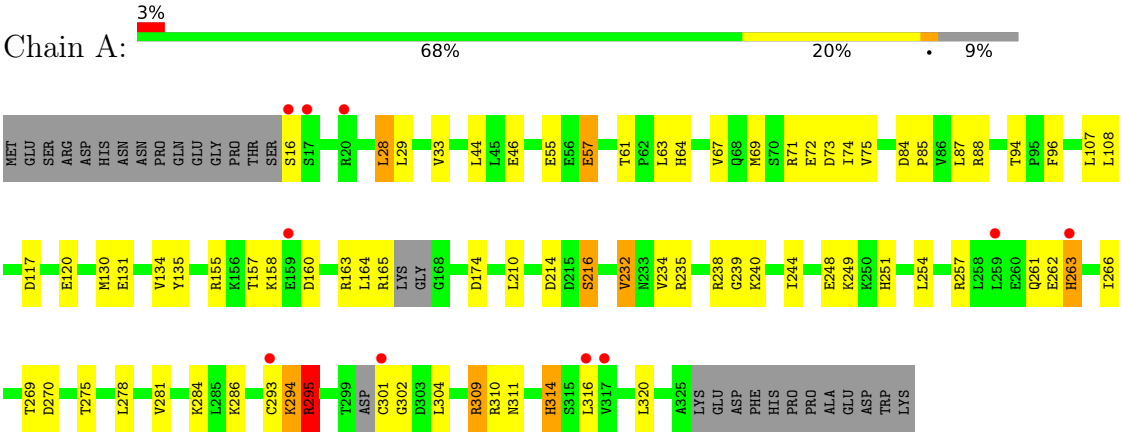
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			67	30	15	19	3		
2	D	1	Total	C	N	O	P	0	0
			67	30	15	19	3		

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.

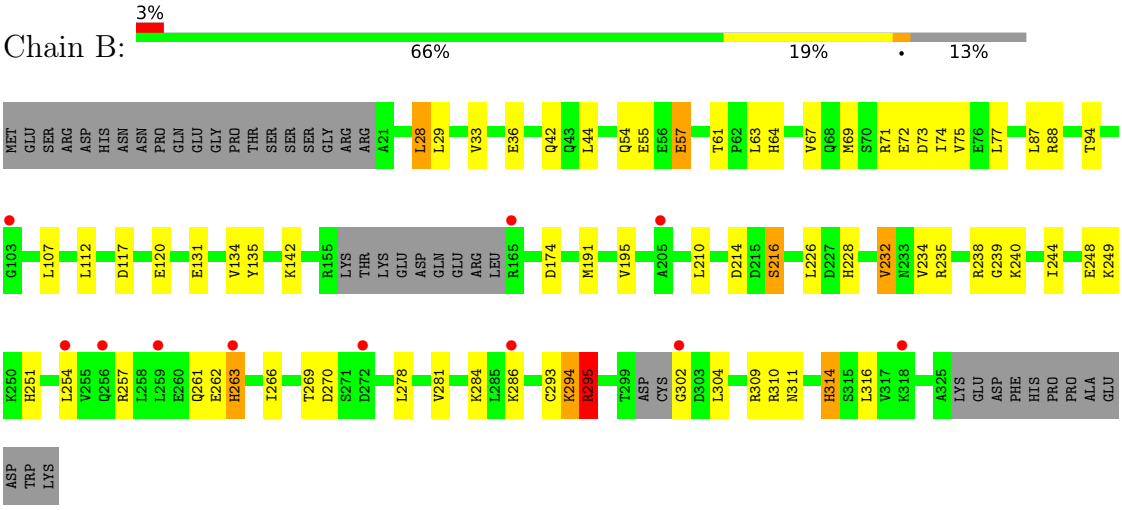
• Molecule 1: 2-5A-dependent ribonuclease

Chain A:



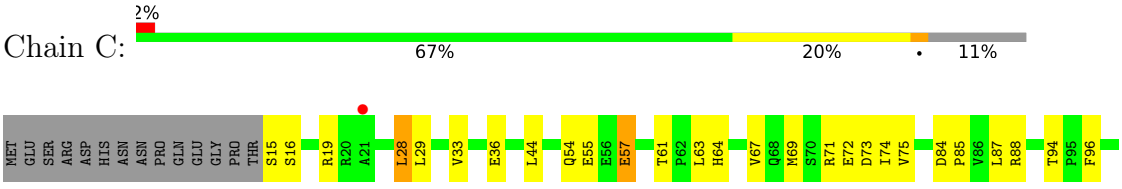
• Molecule 1: 2-5A-dependent ribonuclease

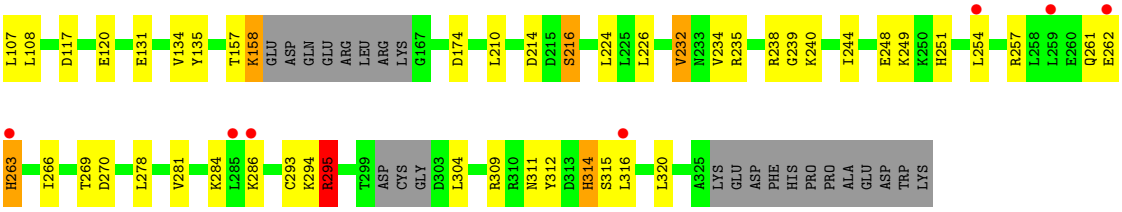
Chain B:



• Molecule 1: 2-5A-dependent ribonuclease

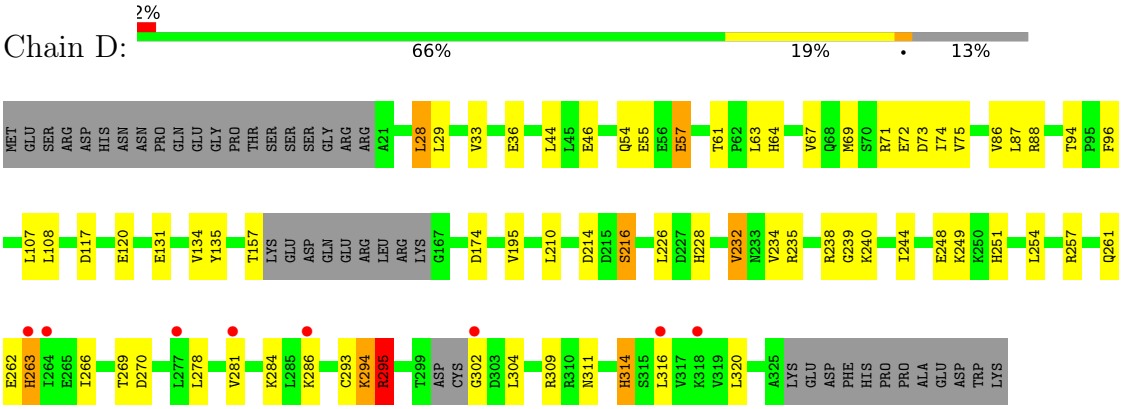
Chain C:





• Molecule 1: 2-5A-dependent ribonuclease

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.98Å 164.11Å 86.22Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	38.75 – 2.80 61.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.75-2.80) 99.9 (61.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.228 , 0.261 0.227 , 0.262	Depositor DCC
R_{free} test set	2117 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.814	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9415	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0774e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 25A

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	0.32	0/2384	0.51	0/3207
1	B	0.32	0/2274	0.49	0/3062
1	C	0.32	0/2319	0.49	0/3121
1	D	0.32	0/2270	0.48	0/3058
All	All	0.32	0/9247	0.49	0/12448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2359	0	2411	65	0
1	B	2249	0	2302	56	0
1	C	2294	0	2350	61	0
1	D	2245	0	2296	58	0
2	A	67	0	31	3	0
2	B	67	0	31	4	0
2	C	67	0	31	2	0
2	D	67	0	31	3	0
All	All	9415	0	9483	232	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 12.

All (232) 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:295:ARG:HG2	1:A:295:ARG:HH11	1.36	0.91
1:B:295:ARG:HH11	1:B:295:ARG:HG2	1.36	0.90
1:D:295:ARG:HG2	1:D:295:ARG:HH11	1.37	0.90
1:A:69:MET:HG2	1:B:314:HIS:CE1	2.07	0.90
1:C:295:ARG:HG2	1:C:295:ARG:HH11	1.37	0.90
1:A:314:HIS:CE1	1:B:69:MET:HG2	2.11	0.85
1:C:314:HIS:CE1	1:D:69:MET:HG2	2.18	0.79
1:B:294:LYS:O	1:B:295:ARG:HG2	1.85	0.77
1:D:294:LYS:O	1:D:295:ARG:HG2	1.85	0.77
1:C:294:LYS:O	1:C:295:ARG:HG2	1.84	0.77
1:D:281:VAL:HG22	1:D:316:LEU:HD21	1.67	0.76
1:A:157:THR:OG1	1:A:160:ASP:HB2	1.86	0.76
1:A:294:LYS:O	1:A:295:ARG:HG2	1.84	0.76
1:A:281:VAL:HG22	1:A:316:LEU:HD21	1.68	0.76
1:B:281:VAL:HG22	1:B:316:LEU:HD21	1.69	0.75
1:C:281:VAL:HG22	1:C:316:LEU:HD21	1.69	0.74
1:D:295:ARG:HH11	1:D:295:ARG:CG	2.01	0.74
1:B:295:ARG:HH11	1:B:295:ARG:CG	2.01	0.73
1:A:295:ARG:HH11	1:A:295:ARG:CG	2.01	0.72
1:C:295:ARG:HH11	1:C:295:ARG:CG	2.02	0.71
1:D:251:HIS:CD2	1:D:254:LEU:H	2.09	0.71
1:B:251:HIS:CD2	1:B:254:LEU:H	2.09	0.70
1:A:61:THR:H	1:A:64:HIS:HD2	1.40	0.69
1:D:251:HIS:HD2	1:D:254:LEU:H	1.40	0.68
1:B:28:LEU:HD13	1:B:44:LEU:HD11	1.75	0.68
1:A:28:LEU:HD13	1:A:44:LEU:HD11	1.74	0.68
1:C:251:HIS:CD2	1:C:254:LEU:H	2.11	0.68
1:B:251:HIS:HD2	1:B:254:LEU:H	1.40	0.67
1:D:28:LEU:HD13	1:D:44:LEU:HD11	1.76	0.67
1:A:251:HIS:CD2	1:A:254:LEU:H	2.13	0.67
1:C:251:HIS:HD2	1:C:254:LEU:H	1.42	0.66
1:D:61:THR:H	1:D:64:HIS:HD2	1.45	0.65
1:C:61:THR:H	1:C:64:HIS:HD2	1.44	0.65
1:C:28:LEU:HD13	1:C:44:LEU:HD11	1.78	0.65
1:B:71:ARG:O	1:B:75:VAL:HG23	1.96	0.64
1:A:251:HIS:HD2	1:A:254:LEU:H	1.43	0.64
1:C:69:MET:HG2	1:D:314:HIS:CE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LEU:O	1:D:67:VAL:HG23	1.99	0.63
1:B:61:THR:H	1:B:64:HIS:HD2	1.47	0.63
1:B:232:VAL:HG11	1:B:261:GLN:HG3	1.82	0.62
1:C:157:THR:O	1:C:158:LYS:HG2	2.00	0.61
1:D:232:VAL:HG11	1:D:261:GLN:HG3	1.83	0.61
1:A:232:VAL:HG11	1:A:261:GLN:HG3	1.82	0.61
1:A:71:ARG:O	1:A:75:VAL:HG23	2.01	0.60
1:C:71:ARG:O	1:C:75:VAL:HG23	2.01	0.60
1:C:232:VAL:HG11	1:C:261:GLN:HG3	1.83	0.60
1:A:163:ARG:O	1:A:164:LEU:HG	2.01	0.59
1:B:63:LEU:O	1:B:67:VAL:HG23	2.02	0.59
1:C:63:LEU:O	1:C:67:VAL:HG23	2.02	0.59
1:D:71:ARG:O	1:D:75:VAL:HG23	2.01	0.59
1:A:63:LEU:O	1:A:67:VAL:HG23	2.03	0.59
1:D:117:ASP:O	1:D:120:GLU:HG2	2.03	0.59
1:D:235:ARG:HD2	1:D:239:GLY:HA2	1.84	0.58
1:A:61:THR:H	1:A:64:HIS:CD2	2.22	0.58
1:A:67:VAL:HG13	1:A:107:LEU:HD13	1.85	0.58
1:A:284:LYS:HG3	1:A:311:ASN:ND2	2.19	0.58
1:D:88:ARG:HG2	1:D:94:THR:HG22	1.85	0.58
1:A:235:ARG:HD2	1:A:239:GLY:HA2	1.86	0.57
1:B:117:ASP:O	1:B:120:GLU:HG2	2.04	0.57
1:C:88:ARG:HG2	1:C:94:THR:HG22	1.86	0.57
1:B:235:ARG:HD2	1:B:239:GLY:HA2	1.85	0.57
1:C:67:VAL:HG13	1:C:107:LEU:HD13	1.87	0.57
1:C:284:LYS:HG3	1:C:311:ASN:ND2	2.20	0.57
1:B:262:GLU:HG3	1:B:263:HIS:CE1	2.40	0.56
1:C:240:LYS:HE3	1:C:248:GLU:OE2	2.05	0.56
1:B:294:LYS:C	1:B:295:ARG:HG2	2.26	0.56
1:C:235:ARG:HD2	1:C:239:GLY:HA2	1.88	0.56
1:B:88:ARG:HG2	1:B:94:THR:HG22	1.88	0.56
1:D:240:LYS:HE3	1:D:248:GLU:OE2	2.06	0.55
1:D:262:GLU:HG3	1:D:263:HIS:CE1	2.41	0.55
1:D:294:LYS:C	1:D:295:ARG:HG2	2.27	0.55
1:A:88:ARG:HG2	1:A:94:THR:HG22	1.89	0.55
1:A:117:ASP:O	1:A:120:GLU:HG2	2.05	0.55
1:A:262:GLU:HG3	1:A:263:HIS:CE1	2.41	0.55
1:B:67:VAL:HG13	1:B:107:LEU:HD13	1.86	0.55
1:B:284:LYS:HG3	1:B:311:ASN:ND2	2.21	0.55
1:D:244:ILE:O	1:D:248:GLU:HG3	2.06	0.55
1:C:262:GLU:HG3	1:C:263:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLU:OE2	2:C:401:25A:N1	2.39	0.55
1:B:131:GLU:OE2	2:B:401:25A:N1	2.40	0.55
1:D:244:ILE:HD13	1:D:270:ASP:HB3	1.89	0.55
1:B:244:ILE:HD13	1:B:270:ASP:HB3	1.88	0.54
1:C:61:THR:H	1:C:64:HIS:CD2	2.25	0.54
1:D:67:VAL:HG13	1:D:107:LEU:HD13	1.87	0.54
1:A:55:GLU:OE2	1:A:57:GLU:HB3	2.08	0.54
1:C:117:ASP:O	1:C:120:GLU:HG2	2.06	0.54
1:D:284:LYS:HG3	1:D:311:ASN:ND2	2.22	0.54
1:A:295:ARG:CG	1:A:295:ARG:NH1	2.66	0.54
1:D:134:VAL:HG22	1:D:174:ASP:HB3	1.88	0.54
1:A:244:ILE:O	1:A:248:GLU:HG3	2.08	0.54
1:A:69:MET:HG2	1:B:314:HIS:NE2	2.21	0.54
1:B:244:ILE:O	1:B:248:GLU:HG3	2.08	0.54
1:C:294:LYS:C	1:C:295:ARG:HG2	2.27	0.54
1:A:240:LYS:HE3	1:A:248:GLU:OE2	2.08	0.54
1:A:294:LYS:C	1:A:295:ARG:HG2	2.27	0.53
1:C:295:ARG:CG	1:C:295:ARG:NH1	2.67	0.53
1:C:55:GLU:OE2	1:C:57:GLU:HB3	2.09	0.53
1:D:131:GLU:OE2	2:D:401:25A:N1	2.42	0.53
1:C:214:ASP:C	1:C:216:SER:H	2.13	0.53
1:D:61:THR:H	1:D:64:HIS:CD2	2.25	0.52
1:A:134:VAL:HG22	1:A:174:ASP:HB3	1.91	0.52
1:B:240:LYS:HE3	1:B:248:GLU:OE2	2.09	0.52
1:B:266:ILE:H	1:B:266:ILE:HD12	1.75	0.52
1:C:244:ILE:HD13	1:C:270:ASP:HB3	1.91	0.52
1:A:244:ILE:HD13	1:A:270:ASP:HB3	1.92	0.52
1:B:135:TYR:OH	2:B:401:25A:N11	2.37	0.52
1:B:55:GLU:OE2	1:B:57:GLU:HB3	2.09	0.51
1:A:160:ASP:OD1	1:A:165:ARG:HD2	2.11	0.51
1:D:266:ILE:HD12	1:D:266:ILE:H	1.76	0.51
1:A:266:ILE:HD12	1:A:266:ILE:H	1.76	0.51
1:B:61:THR:H	1:B:64:HIS:CD2	2.27	0.51
1:D:214:ASP:C	1:D:216:SER:H	2.13	0.51
1:B:214:ASP:C	1:B:216:SER:H	2.13	0.50
1:D:135:TYR:OH	2:D:401:25A:N11	2.39	0.50
1:C:244:ILE:O	1:C:248:GLU:HG3	2.11	0.50
1:A:214:ASP:C	1:A:216:SER:H	2.14	0.50
1:C:266:ILE:HD12	1:C:266:ILE:H	1.77	0.50
1:B:134:VAL:HG22	1:B:174:ASP:HB3	1.93	0.49
1:A:275:THR:HG23	1:A:301:CYS:SG	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:VAL:HG22	1:C:174:ASP:HB3	1.93	0.49
1:A:131:GLU:OE2	2:A:401:25A:N1	2.45	0.49
1:D:55:GLU:OE2	1:D:57:GLU:HB3	2.11	0.49
1:A:293:CYS:C	1:A:295:ARG:H	2.16	0.48
1:C:61:THR:N	1:C:64:HIS:HD2	2.11	0.48
1:A:135:TYR:OH	2:A:401:25A:N11	2.39	0.48
1:D:61:THR:HG21	1:D:87:LEU:HD23	1.95	0.47
1:A:262:GLU:HG3	1:A:263:HIS:ND1	2.28	0.47
1:A:304:LEU:HD13	1:A:320:LEU:HD22	1.96	0.47
1:C:293:CYS:C	1:C:295:ARG:H	2.17	0.47
1:B:262:GLU:HG3	1:B:263:HIS:ND1	2.29	0.47
1:A:61:THR:HG21	1:A:87:LEU:HD23	1.96	0.47
1:C:29:LEU:O	1:C:33:VAL:HG23	2.15	0.47
1:C:304:LEU:HD13	1:C:320:LEU:HD22	1.97	0.47
1:D:29:LEU:O	1:D:33:VAL:HG23	2.15	0.47
1:C:262:GLU:HG3	1:C:263:HIS:ND1	2.29	0.47
1:D:262:GLU:HG3	1:D:263:HIS:ND1	2.29	0.47
1:A:165:ARG:NH2	1:D:86:VAL:HG23	2.29	0.46
1:A:286:LYS:NZ	1:A:286:LYS:HB2	2.31	0.46
1:D:214:ASP:HB3	1:D:216:SER:OG	2.15	0.46
1:D:238:ARG:C	1:D:240:LYS:H	2.19	0.46
1:B:29:LEU:O	1:B:33:VAL:HG23	2.16	0.46
1:C:286:LYS:HB2	1:C:286:LYS:NZ	2.31	0.46
1:A:61:THR:N	1:A:64:HIS:HD2	2.09	0.45
1:A:310:ARG:HG2	2:B:401:25A:H22'	1.98	0.45
1:C:135:TYR:OH	2:C:401:25A:N11	2.41	0.45
1:A:29:LEU:O	1:A:33:VAL:HG23	2.16	0.45
1:D:295:ARG:CG	1:D:295:ARG:NH1	2.67	0.45
1:C:96:PHE:CE1	1:C:108:LEU:HD22	2.52	0.45
1:C:244:ILE:CD1	1:C:270:ASP:HB3	2.46	0.45
1:A:73:ASP:OD1	1:A:74:ILE:N	2.50	0.45
1:B:210:LEU:O	1:B:249:LYS:HE2	2.16	0.45
1:B:238:ARG:C	1:B:240:LYS:H	2.20	0.45
1:D:286:LYS:HB2	1:D:286:LYS:NZ	2.32	0.45
1:D:61:THR:OG1	1:D:64:HIS:CD2	2.69	0.45
1:D:293:CYS:C	1:D:295:ARG:H	2.18	0.45
1:D:304:LEU:HD13	1:D:320:LEU:HD22	1.98	0.45
1:B:295:ARG:CG	1:B:295:ARG:NH1	2.67	0.45
1:C:61:THR:HG21	1:C:87:LEU:HD23	1.98	0.45
1:D:61:THR:N	1:D:64:HIS:HD2	2.11	0.45
1:A:69:MET:CG	1:B:314:HIS:CE1	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASP:HB3	1:B:216:SER:OG	2.17	0.44
1:C:73:ASP:OD1	1:C:74:ILE:N	2.51	0.44
1:C:72:GLU:H	1:C:72:GLU:HG3	1.60	0.44
1:D:73:ASP:OD1	1:D:74:ILE:N	2.51	0.44
1:D:302:GLY:C	1:D:304:LEU:H	2.21	0.44
1:B:293:CYS:C	1:B:295:ARG:H	2.19	0.44
1:A:158:LYS:C	1:A:160:ASP:H	2.21	0.43
1:C:214:ASP:HB3	1:C:216:SER:OG	2.17	0.43
1:A:275:THR:CG2	1:A:301:CYS:SG	3.06	0.43
1:B:286:LYS:HB2	1:B:286:LYS:NZ	2.33	0.43
1:C:238:ARG:C	1:C:240:LYS:H	2.20	0.43
1:C:63:LEU:HD11	1:C:75:VAL:HG13	2.00	0.43
1:A:238:ARG:C	1:A:240:LYS:H	2.20	0.43
1:B:244:ILE:CD1	1:B:270:ASP:HB3	2.46	0.43
1:C:28:LEU:O	1:C:28:LEU:HD22	2.19	0.43
1:D:244:ILE:CD1	1:D:270:ASP:HB3	2.46	0.43
1:A:63:LEU:HD11	1:A:75:VAL:HG13	2.00	0.43
1:A:302:GLY:C	1:A:304:LEU:H	2.21	0.43
1:A:210:LEU:O	1:A:249:LYS:HE2	2.19	0.43
1:B:61:THR:N	1:B:64:HIS:HD2	2.13	0.43
1:C:226:LEU:HD21	1:C:232:VAL:HG13	2.00	0.43
1:D:210:LEU:O	1:D:249:LYS:HE2	2.18	0.43
1:D:72:GLU:H	1:D:72:GLU:HG3	1.58	0.43
1:C:29:LEU:HA	1:C:44:LEU:HD13	2.01	0.42
1:A:96:PHE:CE1	1:A:108:LEU:HD22	2.54	0.42
1:B:36:GLU:HB3	1:B:71:ARG:HH12	1.83	0.42
1:C:240:LYS:HE3	1:C:248:GLU:CD	2.39	0.42
1:C:226:LEU:CD2	1:C:232:VAL:HG13	2.49	0.42
1:B:302:GLY:C	1:B:304:LEU:H	2.22	0.42
1:D:240:LYS:HE3	1:D:248:GLU:CD	2.39	0.42
1:A:214:ASP:HB3	1:A:216:SER:OG	2.18	0.42
1:A:314:HIS:CE1	1:B:69:MET:CG	2.95	0.42
1:D:226:LEU:HD21	1:D:232:VAL:HG13	2.01	0.42
1:B:195:VAL:HG11	1:B:228:HIS:O	2.20	0.42
1:C:84:ASP:HA	1:C:85:PRO:HD3	1.74	0.42
1:D:88:ARG:HG2	1:D:94:THR:CG2	2.48	0.42
1:A:240:LYS:HE3	1:A:248:GLU:CD	2.40	0.42
1:B:54:GLN:HG2	1:B:61:THR:HG22	2.02	0.42
2:A:401:25A:H22	1:B:310:ARG:HA	2.02	0.42
1:C:15:SER:O	1:C:19:ARG:N	2.39	0.42
1:D:235:ARG:HH11	1:D:239:GLY:HA2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:LEU:CD2	1:D:232:VAL:HG13	2.50	0.41
1:A:84:ASP:HA	1:A:85:PRO:HD3	1.73	0.41
1:A:244:ILE:CD1	1:A:270:ASP:HB3	2.50	0.41
1:D:240:LYS:HE3	1:D:248:GLU:OE1	2.20	0.41
1:A:235:ARG:HH11	1:A:239:GLY:HA2	1.84	0.41
1:C:54:GLN:HG2	1:C:61:THR:HG22	2.01	0.41
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.95	0.41
1:D:54:GLN:HG2	1:D:61:THR:HG22	2.02	0.41
1:A:29:LEU:HA	1:A:44:LEU:HD13	2.03	0.41
1:A:130:MET:SD	1:A:155:ARG:HG2	2.61	0.41
1:A:309:ARG:HG2	2:B:401:25A:N26	2.36	0.41
1:B:72:GLU:H	1:B:72:GLU:HG3	1.60	0.41
1:B:142:LYS:HA	1:B:191:MET:HE2	2.03	0.41
1:D:36:GLU:HB3	1:D:71:ARG:HH12	1.84	0.41
1:C:131:GLU:OE1	1:C:131:GLU:HA	2.21	0.41
1:B:42:GLN:HG3	1:B:77:LEU:HD21	2.03	0.41
1:B:73:ASP:OD1	1:B:74:ILE:N	2.53	0.41
1:C:36:GLU:HB3	1:C:71:ARG:HH12	1.86	0.41
1:C:210:LEU:O	1:C:249:LYS:HE2	2.21	0.41
1:C:312:TYR:CE2	2:D:401:25A:C12	3.04	0.41
1:D:195:VAL:HG11	1:D:228:HIS:O	2.21	0.41
1:A:240:LYS:HE3	1:A:248:GLU:OE1	2.21	0.40
1:B:28:LEU:O	1:B:28:LEU:HD22	2.22	0.40
1:B:226:LEU:CD2	1:B:232:VAL:HG13	2.51	0.40
1:C:224:LEU:HD23	1:C:224:LEU:HA	1.90	0.40
1:A:131:GLU:HA	1:A:131:GLU:OE1	2.21	0.40
1:B:61:THR:HG21	1:B:87:LEU:HD23	2.02	0.40
1:D:96:PHE:CE1	1:D:108:LEU:HD22	2.56	0.40
1:D:131:GLU:HA	1:D:131:GLU:OE1	2.20	0.40
1:C:235:ARG:HH11	1:C:239:GLY:HA2	1.85	0.40
1:C:286:LYS:CE	1:C:315:SER:HB3	2.51	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	301/337 (89%)	279 (93%)	20 (7%)	2 (1%)	22	53
1	B	288/337 (86%)	268 (93%)	18 (6%)	2 (1%)	22	53
1	C	294/337 (87%)	275 (94%)	18 (6%)	1 (0%)	41	72
1	D	288/337 (86%)	269 (93%)	17 (6%)	2 (1%)	22	53
All	All	1171/1348 (87%)	1091 (93%)	73 (6%)	7 (1%)	25	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	ARG
1	B	295	ARG
1	C	295	ARG
1	D	295	ARG
1	A	294	LYS
1	B	294	LYS
1	D	294	LYS

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	250/277 (90%)	235 (94%)	15 (6%)	19	48
1	B	237/277 (86%)	225 (95%)	12 (5%)	24	55
1	C	243/277 (88%)	229 (94%)	14 (6%)	20	50
1	D	237/277 (86%)	223 (94%)	14 (6%)	19	49
All	All	967/1108 (87%)	912 (94%)	55 (6%)	20	50

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER

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Mol	Chain	Res	Type
1	A	28	LEU
1	A	46	GLU
1	A	57	GLU
1	A	72	GLU
1	A	216	SER
1	A	232	VAL
1	A	234	VAL
1	A	257	ARG
1	A	263	HIS
1	A	269	THR
1	A	278	LEU
1	A	295	ARG
1	A	309	ARG
1	A	314	HIS
1	B	28	LEU
1	B	57	GLU
1	B	216	SER
1	B	232	VAL
1	B	234	VAL
1	B	257	ARG
1	B	263	HIS
1	B	269	THR
1	B	278	LEU
1	B	295	ARG
1	B	309	ARG
1	B	314	HIS
1	C	16	SER
1	C	28	LEU
1	C	57	GLU
1	C	158	LYS
1	C	216	SER
1	C	232	VAL
1	C	234	VAL
1	C	257	ARG
1	C	263	HIS
1	C	269	THR
1	C	278	LEU
1	C	295	ARG
1	C	309	ARG
1	C	314	HIS
1	D	28	LEU
1	D	46	GLU

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Mol	Chain	Res	Type
1	D	57	GLU
1	D	157	THR
1	D	216	SER
1	D	232	VAL
1	D	234	VAL
1	D	257	ARG
1	D	263	HIS
1	D	269	THR
1	D	278	LEU
1	D	295	ARG
1	D	309	ARG
1	D	314	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	81	HIS
1	A	180	HIS
1	A	208	HIS
1	A	251	HIS
1	A	314	HIS
1	A	323	HIS
1	B	64	HIS
1	B	81	HIS
1	B	180	HIS
1	B	208	HIS
1	B	251	HIS
1	B	314	HIS
1	B	323	HIS
1	C	64	HIS
1	C	81	HIS
1	C	208	HIS
1	C	251	HIS
1	C	314	HIS
1	C	323	HIS
1	D	64	HIS
1	D	81	HIS
1	D	180	HIS
1	D	208	HIS
1	D	251	HIS
1	D	314	HIS

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Mol	Chain	Res	Type
1	D	323	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	25A	A	401	-	64,75,75	3.34	26 (40%)	75,116,116	1.83	17 (22%)
2	25A	D	401	-	64,75,75	3.33	26 (40%)	75,116,116	1.80	17 (22%)
2	25A	C	401	-	64,75,75	3.32	25 (39%)	75,116,116	1.78	16 (21%)
2	25A	B	401	-	64,75,75	3.35	25 (39%)	75,116,116	1.79	16 (21%)

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
2	25A	A	401	-	-	10/28/88/88	0/9/9/9
2	25A	D	401	-	-	10/28/88/88	0/9/9/9
2	25A	C	401	-	-	9/28/88/88	0/9/9/9
2	25A	B	401	-	-	9/28/88/88	0/9/9/9

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	25A	C8-N7	9.60	1.51	1.34
2	C	401	25A	C8-N7	9.58	1.51	1.34
2	A	401	25A	C8-N7	9.48	1.51	1.34
2	D	401	25A	C14-N13	9.48	1.48	1.35
2	D	401	25A	C8-N7	9.48	1.51	1.34
2	B	401	25A	C14-N13	9.35	1.48	1.35
2	C	401	25A	C2-N3	9.20	1.46	1.32
2	B	401	25A	C2-N3	9.17	1.46	1.32
2	A	401	25A	C14-N13	9.00	1.48	1.35
2	D	401	25A	C2-N3	8.99	1.46	1.32
2	C	401	25A	C14-N13	8.94	1.48	1.35
2	A	401	25A	C2-N3	8.88	1.46	1.32
2	C	401	25A	C22-N23	8.46	1.45	1.32
2	B	401	25A	C22-N23	8.28	1.45	1.32
2	A	401	25A	C22-N23	8.26	1.45	1.32
2	D	401	25A	C22-N23	8.11	1.45	1.32
2	B	401	25A	O4'-C1'	7.39	1.51	1.41
2	B	401	25A	OE'-CB'	7.33	1.51	1.41
2	C	401	25A	OE'-CB'	7.31	1.51	1.41
2	A	401	25A	O4'-C1'	7.21	1.51	1.41
2	A	401	25A	OE'-CB'	7.17	1.51	1.41
2	D	401	25A	OE'-CB'	6.88	1.50	1.41
2	C	401	25A	O4'-C1'	6.86	1.50	1.41
2	D	401	25A	O4'-C1'	6.63	1.50	1.41
2	A	401	25A	OO'-CL'	6.45	1.50	1.41
2	D	401	25A	C18-N17	6.41	1.46	1.34
2	A	401	25A	C18-N17	6.23	1.45	1.34
2	C	401	25A	C18-N17	6.20	1.45	1.34
2	B	401	25A	C18-N17	6.18	1.45	1.34
2	D	401	25A	OO'-CL'	6.17	1.49	1.41
2	C	401	25A	OO'-CL'	6.12	1.49	1.41
2	B	401	25A	OO'-CL'	5.94	1.49	1.41
2	D	401	25A	C4-N3	5.71	1.43	1.35
2	A	401	25A	C4-N3	5.62	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	25A	C4-N3	5.57	1.43	1.35
2	B	401	25A	C4-N3	5.47	1.43	1.35
2	D	401	25A	C28-N27	4.28	1.42	1.34
2	A	401	25A	C28-N27	4.26	1.42	1.34
2	C	401	25A	C28-N27	4.09	1.42	1.34
2	B	401	25A	C28-N27	4.08	1.42	1.34
2	C	401	25A	C2-N1	4.04	1.41	1.33
2	B	401	25A	C2-N1	3.95	1.41	1.33
2	D	401	25A	C2-N1	3.88	1.41	1.33
2	A	401	25A	C2-N1	3.82	1.41	1.33
2	D	401	25A	C24-N23	3.41	1.40	1.35
2	B	401	25A	C15-N17	3.37	1.52	1.39
2	A	401	25A	C24-N23	3.33	1.40	1.35
2	C	401	25A	C15-N17	3.23	1.51	1.39
2	D	401	25A	C15-N17	3.22	1.51	1.39
2	A	401	25A	C15-N17	3.12	1.51	1.39
2	B	401	25A	C6-N6	3.03	1.45	1.34
2	C	401	25A	C24-N23	2.95	1.39	1.35
2	A	401	25A	C12-N13	2.95	1.36	1.32
2	D	401	25A	C6-N6	2.94	1.44	1.34
2	B	401	25A	C12-N13	2.94	1.36	1.32
2	A	401	25A	OE'-CE'	2.94	1.51	1.45
2	A	401	25A	C6-N6	2.93	1.44	1.34
2	C	401	25A	C6-N6	2.92	1.44	1.34
2	B	401	25A	C24-N23	2.90	1.39	1.35
2	D	401	25A	C26-N26	2.90	1.44	1.34
2	C	401	25A	C26-N26	2.86	1.44	1.34
2	D	401	25A	C12-N13	2.83	1.36	1.32
2	B	401	25A	C22-N21	2.82	1.39	1.33
2	A	401	25A	C26-N26	2.81	1.44	1.34
2	A	401	25A	C16-N11	2.79	1.49	1.37
2	A	401	25A	C16-N16	2.79	1.44	1.34
2	B	401	25A	C26-N26	2.76	1.44	1.34
2	D	401	25A	C16-N11	2.73	1.49	1.37
2	C	401	25A	C16-N16	2.73	1.44	1.34
2	B	401	25A	OE'-CE'	2.72	1.51	1.45
2	D	401	25A	C3'-C2'	-2.72	1.46	1.52
2	D	401	25A	C16-N16	2.68	1.43	1.34
2	B	401	25A	C16-N16	2.65	1.43	1.34
2	D	401	25A	OE'-CE'	2.64	1.50	1.45
2	D	401	25A	C22-N21	2.64	1.38	1.33
2	C	401	25A	C16-N11	2.63	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	25A	C3'-C2'	-2.63	1.47	1.52
2	A	401	25A	C22-N21	2.60	1.38	1.33
2	C	401	25A	C12-N13	2.60	1.36	1.32
2	C	401	25A	OE'-CE'	2.60	1.50	1.45
2	C	401	25A	C22-N21	2.59	1.38	1.33
2	B	401	25A	C16-N11	2.58	1.48	1.37
2	C	401	25A	C3'-C2'	-2.47	1.47	1.52
2	B	401	25A	C3'-C2'	-2.39	1.47	1.52
2	D	401	25A	C12-N11	2.38	1.38	1.33
2	B	401	25A	C12-N11	2.35	1.38	1.33
2	A	401	25A	C12-N11	2.33	1.38	1.33
2	A	401	25A	P-O5'	-2.25	1.53	1.60
2	B	401	25A	CD'-CC'	-2.18	1.48	1.52
2	D	401	25A	CD'-CC'	-2.18	1.48	1.52
2	C	401	25A	P-O5'	-2.17	1.53	1.60
2	D	401	25A	C6-N1	2.17	1.46	1.37
2	C	401	25A	C6-N1	2.14	1.46	1.37
2	B	401	25A	C6-N1	2.13	1.46	1.37
2	C	401	25A	CD'-CC'	-2.12	1.48	1.52
2	B	401	25A	P-O5'	-2.12	1.53	1.60
2	C	401	25A	O3'-C3'	-2.09	1.38	1.43
2	D	401	25A	P2-OC'	-2.08	1.55	1.60
2	A	401	25A	CD'-CC'	-2.08	1.48	1.52
2	A	401	25A	O3'-C3'	-2.05	1.38	1.43
2	A	401	25A	C6-N1	2.04	1.46	1.37
2	D	401	25A	P-O5'	-2.03	1.53	1.60

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	25A	N13-C12-N11	-5.69	119.78	128.68
2	B	401	25A	N3-C2-N1	-5.58	119.96	128.68
2	A	401	25A	N13-C12-N11	-5.54	120.01	128.68
2	C	401	25A	N13-C12-N11	-5.53	120.03	128.68
2	A	401	25A	N3-C2-N1	-5.53	120.04	128.68
2	D	401	25A	N3-C2-N1	-5.44	120.17	128.68
2	C	401	25A	N23-C22-N21	-5.35	120.32	128.68
2	C	401	25A	N3-C2-N1	-5.34	120.33	128.68
2	A	401	25A	N23-C22-N21	-5.34	120.33	128.68
2	B	401	25A	N13-C12-N11	-5.33	120.35	128.68
2	B	401	25A	N23-C22-N21	-5.05	120.79	128.68
2	D	401	25A	N23-C22-N21	-4.99	120.87	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	25A	O4'-C1'-C2'	-3.70	100.16	106.59
2	C	401	25A	O4'-C1'-C2'	-3.51	100.50	106.59
2	D	401	25A	O4'-C1'-C2'	-3.45	100.60	106.59
2	B	401	25A	O4'-C1'-C2'	-3.44	100.63	106.59
2	A	401	25A	OD'-CD'-CE'	3.17	120.23	111.05
2	D	401	25A	OD'-CD'-CE'	3.16	120.18	111.05
2	B	401	25A	OD'-CD'-CE'	3.15	120.17	111.05
2	C	401	25A	OD'-CD'-CE'	3.11	120.03	111.05
2	A	401	25A	OE'-CE'-CF'	3.09	119.55	109.37
2	B	401	25A	O4'-C4'-C5'	3.06	119.44	109.37
2	D	401	25A	OC'-CC'-CB'	3.05	121.09	110.10
2	A	401	25A	O4'-C4'-C5'	3.04	119.37	109.37
2	D	401	25A	O3'-C3'-C4'	2.99	119.69	111.05
2	A	401	25A	O2'-C2'-C1'	2.97	120.79	110.10
2	C	401	25A	O3'-C3'-C2'	2.95	119.54	111.17
2	A	401	25A	O3'-C3'-C4'	2.92	119.49	111.05
2	B	401	25A	O3'-C3'-C2'	2.92	119.45	111.17
2	D	401	25A	ON'-CN'-CO'	2.91	119.47	111.05
2	C	401	25A	O4'-C4'-C5'	2.90	118.93	109.37
2	C	401	25A	OC'-CC'-CB'	2.90	120.54	110.10
2	C	401	25A	OE'-CE'-CF'	2.86	118.80	109.37
2	B	401	25A	ON'-CN'-CO'	2.86	119.32	111.05
2	D	401	25A	O2'-C2'-C1'	2.86	120.40	110.10
2	A	401	25A	OC'-CC'-CB'	2.82	120.26	110.10
2	B	401	25A	O2'-C2'-C1'	2.82	120.24	110.10
2	A	401	25A	ON'-CN'-CM'	2.76	120.76	111.82
2	B	401	25A	O3'-C3'-C4'	2.76	119.03	111.05
2	A	401	25A	O3'-C3'-C2'	2.75	118.97	111.17
2	B	401	25A	OE'-CE'-CF'	2.75	118.41	109.37
2	C	401	25A	O2'-C2'-C1'	2.74	119.96	110.10
2	A	401	25A	ON'-CN'-CO'	2.71	118.87	111.05
2	D	401	25A	O4'-C4'-C5'	2.70	118.27	109.37
2	D	401	25A	CN'-CM'-CL'	2.70	105.04	100.98
2	D	401	25A	O3'-C3'-C2'	2.69	118.81	111.17
2	B	401	25A	OC'-CC'-CB'	2.69	119.78	110.10
2	C	401	25A	ON'-CN'-CO'	2.67	118.77	111.05
2	B	401	25A	CN'-CM'-CL'	2.66	104.98	100.98
2	D	401	25A	OE'-CE'-CF'	2.65	118.09	109.37
2	C	401	25A	ON'-CN'-CM'	2.62	120.31	111.82
2	B	401	25A	ON'-CN'-CM'	2.61	120.28	111.82
2	C	401	25A	O3'-C3'-C4'	2.60	118.57	111.05
2	D	401	25A	ON'-CN'-CM'	2.56	120.09	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	25A	OO'-CO'-CP'	2.54	117.72	109.37
2	A	401	25A	CN'-CM'-CL'	2.52	104.77	100.98
2	C	401	25A	CN'-CM'-CL'	2.45	104.66	100.98
2	A	401	25A	OO'-CO'-CP'	2.41	117.31	109.37
2	C	401	25A	OM'-CM'-CN'	2.39	119.57	111.82
2	A	401	25A	OM'-CM'-CN'	2.37	119.50	111.82
2	D	401	25A	OM'-CM'-CN'	2.36	119.47	111.82
2	B	401	25A	OO'-CO'-CP'	2.31	116.98	109.37
2	B	401	25A	OM'-CM'-CN'	2.22	119.00	111.82
2	C	401	25A	OO'-CO'-CP'	2.20	116.62	109.37
2	D	401	25A	C24-C25-N27	-2.16	107.14	109.40
2	A	401	25A	OM'-CM'-CL'	2.06	118.46	110.85

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	25A	C2'-O2'-P1-OBP
2	A	401	25A	CF'-OF'-P1-OCP
2	A	401	25A	CP'-OP'-P2-OLP
2	B	401	25A	CF'-OF'-P1-OCP
2	B	401	25A	CP'-OP'-P2-OLP
2	C	401	25A	CF'-OF'-P1-OCP
2	C	401	25A	CP'-OP'-P2-OLP
2	D	401	25A	C2'-O2'-P1-OBP
2	D	401	25A	CF'-OF'-P1-OCP
2	D	401	25A	CP'-OP'-P2-OLP
2	A	401	25A	CP'-OP'-P2-OC'
2	B	401	25A	CP'-OP'-P2-OC'
2	C	401	25A	CP'-OP'-P2-OC'
2	D	401	25A	CP'-OP'-P2-OC'
2	C	401	25A	CN'-CO'-CP'-OP'
2	A	401	25A	CN'-CO'-CP'-OP'
2	D	401	25A	CN'-CO'-CP'-OP'
2	B	401	25A	CN'-CO'-CP'-OP'
2	A	401	25A	C2'-O2'-P1-OCP
2	B	401	25A	C2'-O2'-P1-OBP
2	B	401	25A	C2'-O2'-P1-OCP
2	C	401	25A	C2'-O2'-P1-OBP
2	C	401	25A	C2'-O2'-P1-OCP
2	D	401	25A	C2'-O2'-P1-OCP
2	A	401	25A	OE'-CE'-CF'-OF'

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Mol	Chain	Res	Type	Atoms
2	D	401	25A	OE'-CE'-CF'-OF'
2	A	401	25A	CP'-OP'-P2-OMP
2	B	401	25A	CP'-OP'-P2-OMP
2	C	401	25A	CP'-OP'-P2-OMP
2	D	401	25A	CP'-OP'-P2-OMP
2	C	401	25A	OE'-CE'-CF'-OF'
2	B	401	25A	OE'-CE'-CF'-OF'
2	A	401	25A	C2'-O2'-P1-OF'
2	C	401	25A	C2'-O2'-P1-OF'
2	D	401	25A	C2'-O2'-P1-OF'
2	B	401	25A	C2'-O2'-P1-OF'
2	A	401	25A	CF'-OF'-P1-O2'
2	D	401	25A	CF'-OF'-P1-O2'

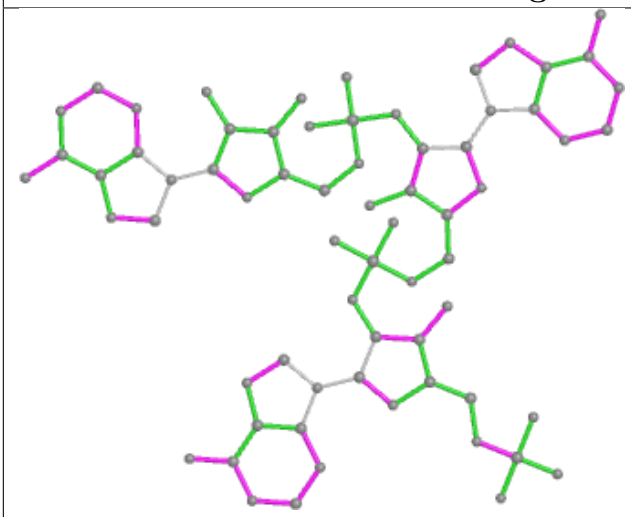
There are no ring outliers.

4 monomers are involved in 12 short contacts:

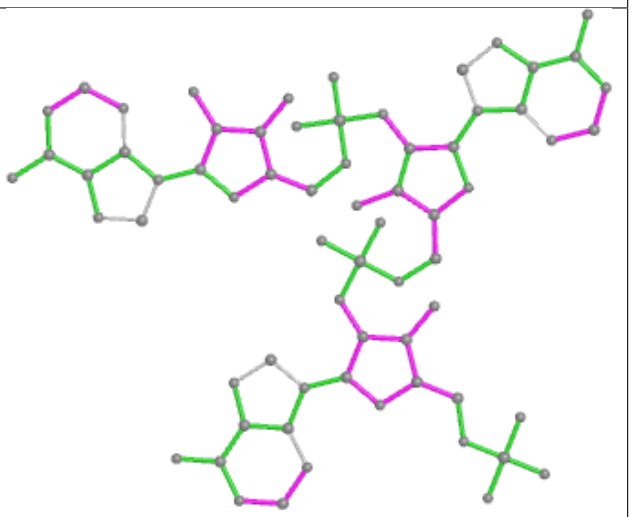
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	25A	3	0
2	D	401	25A	3	0
2	C	401	25A	2	0
2	B	401	25A	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

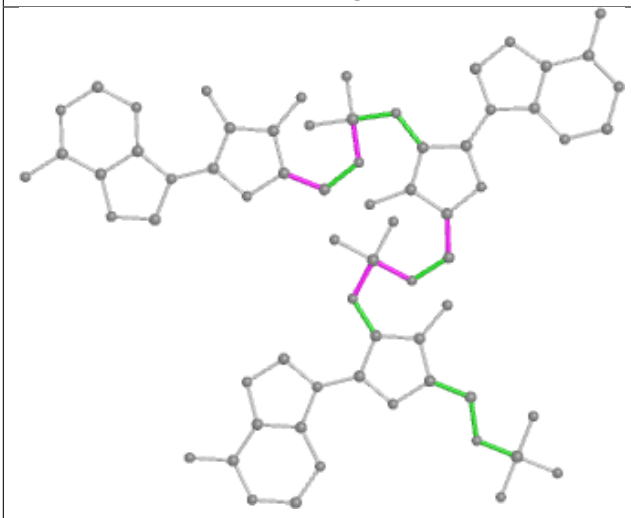
Ligand 25A A 401



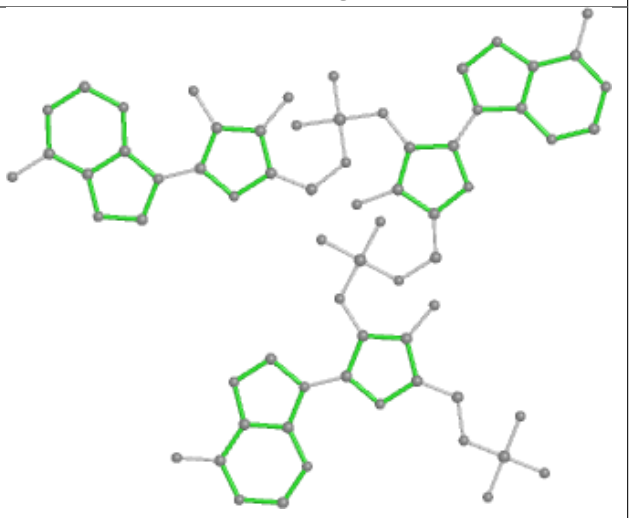
Bond lengths



Bond angles

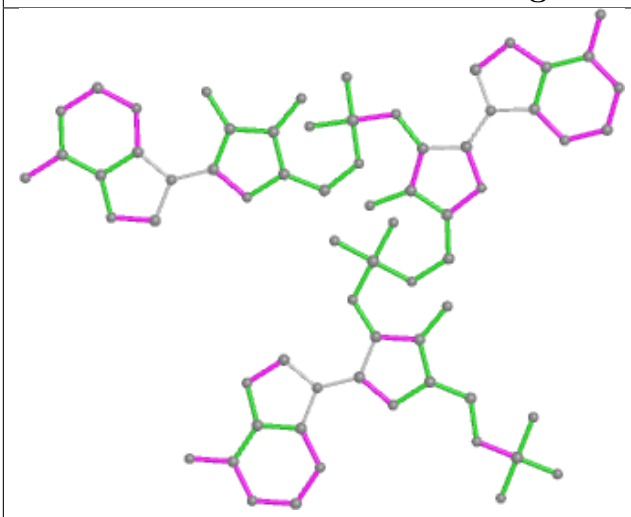


Torsions

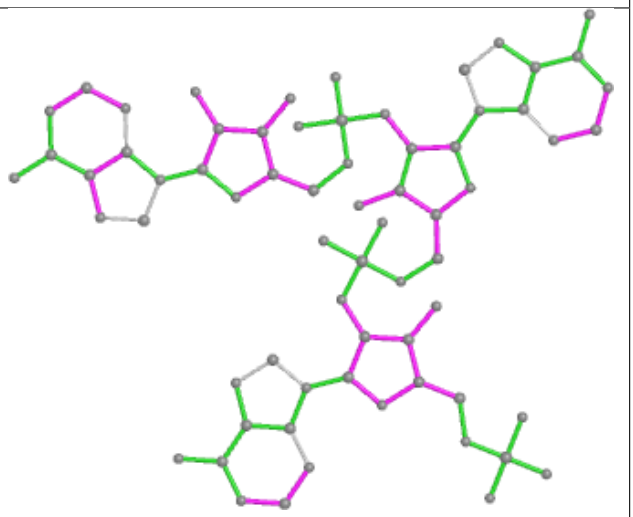


Rings

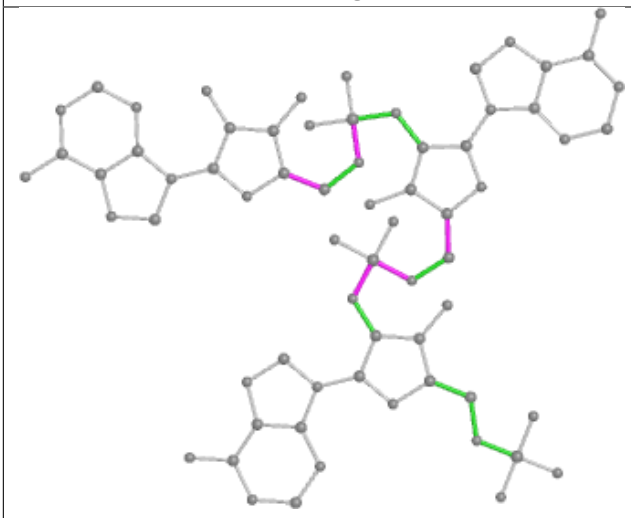
Ligand 25A D 401



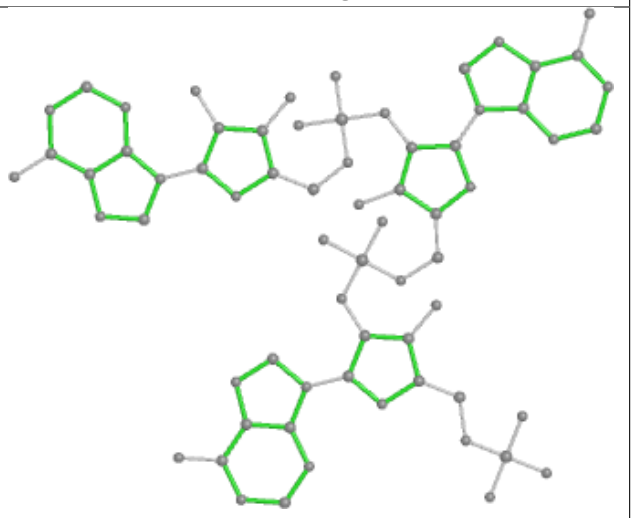
Bond lengths



Bond angles

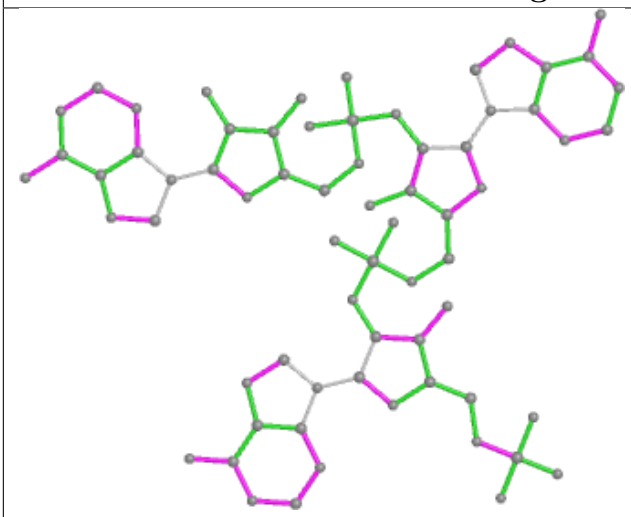


Torsions

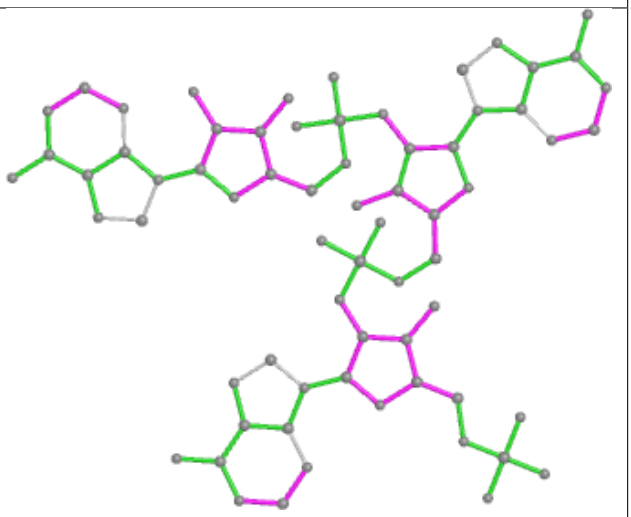


Rings

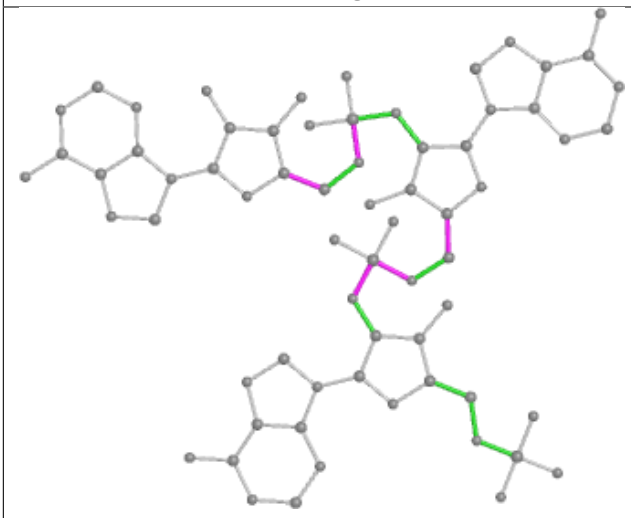
Ligand 25A C 401



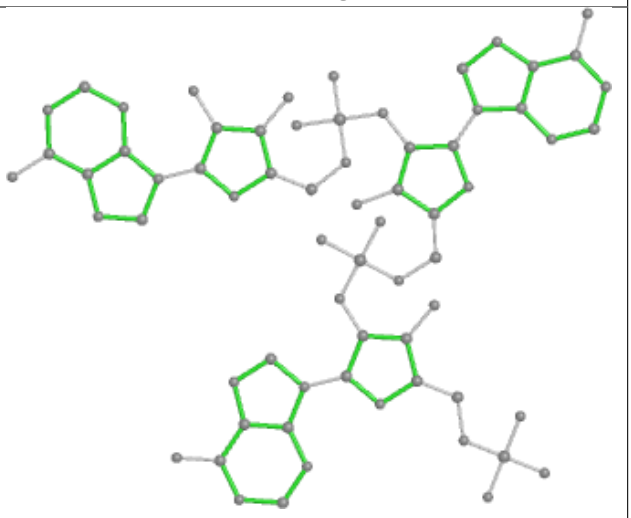
Bond lengths



Bond angles

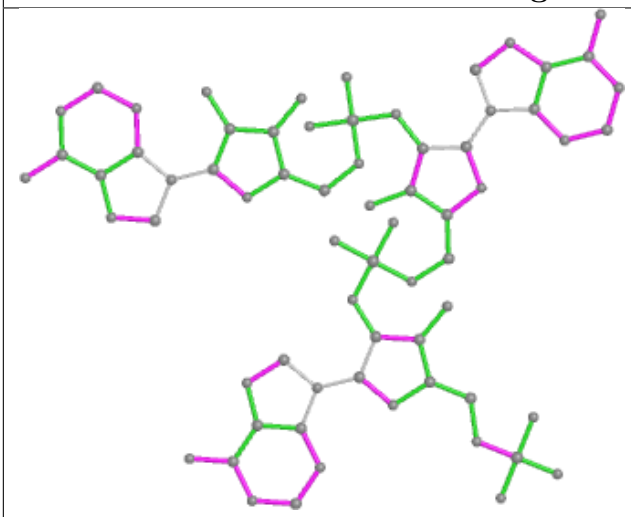


Torsions

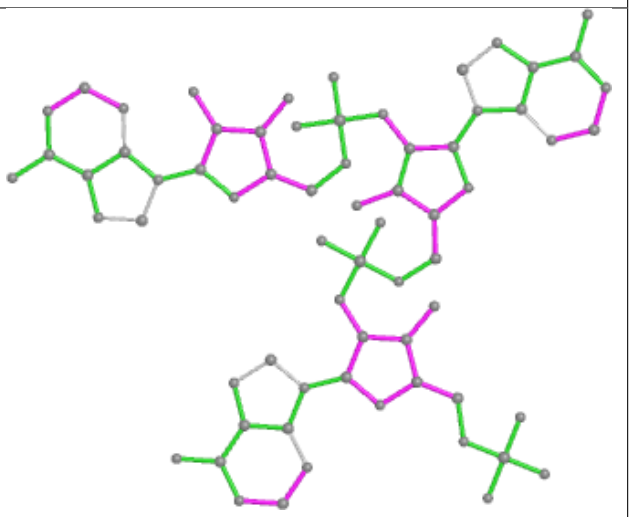


Rings

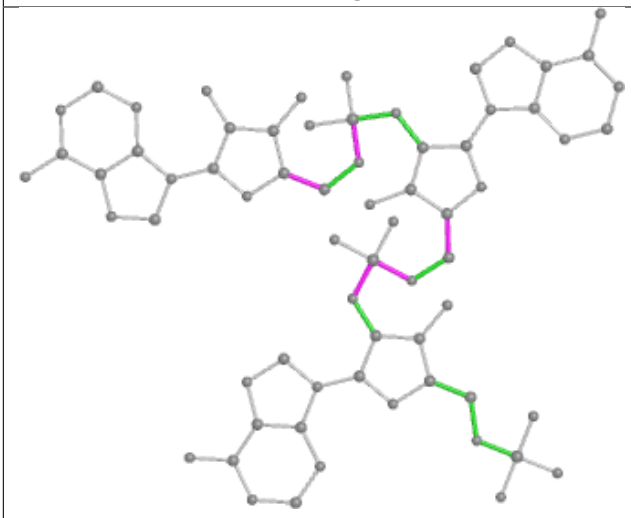
Ligand 25A B 401



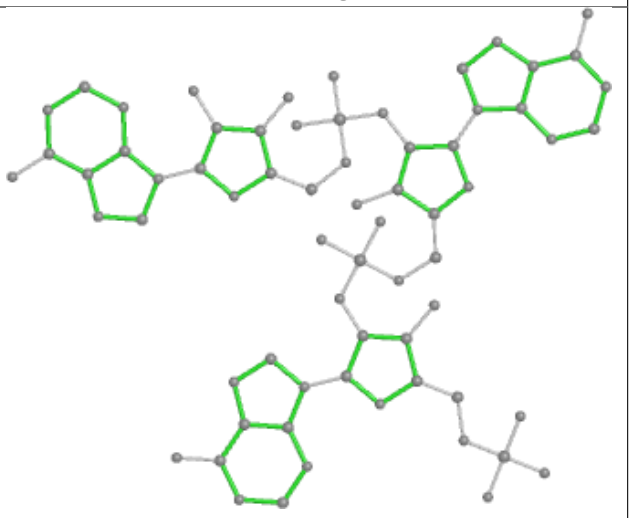
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	307/337 (91%)	0.30	10 (3%)	46	36	35, 63, 117, 165	0
1	B	294/337 (87%)	0.29	11 (3%)	41	31	36, 62, 112, 161	0
1	C	300/337 (89%)	0.24	8 (2%)	54	44	36, 63, 115, 163	0
1	D	294/337 (87%)	0.20	8 (2%)	54	44	38, 65, 112, 161	0
All	All	1195/1348 (88%)	0.26	37 (3%)	49	39	35, 64, 113, 165	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	SER	6.5
1	B	302	GLY	5.9
1	A	16	SER	5.8
1	A	263	HIS	5.1
1	A	301	CYS	4.7
1	A	316	LEU	4.6
1	D	302	GLY	4.1
1	C	286	LYS	3.4
1	C	263	HIS	3.3
1	B	259	LEU	3.1
1	A	20	ARG	3.1
1	A	159	GLU	2.9
1	D	263	HIS	2.9
1	A	259	LEU	2.9
1	D	286	LYS	2.8
1	B	263	HIS	2.8
1	D	277	LEU	2.8
1	D	316	LEU	2.7
1	C	259	LEU	2.7
1	B	286	LYS	2.7
1	B	256	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	272	ASP	2.6
1	B	318	LYS	2.6
1	B	254	LEU	2.6
1	C	285	LEU	2.5
1	B	205	ALA	2.4
1	D	264	ILE	2.4
1	D	281	VAL	2.4
1	C	316	LEU	2.3
1	B	165	ARG	2.3
1	C	254	LEU	2.3
1	A	293	CYS	2.2
1	C	21	ALA	2.2
1	D	318	LYS	2.2
1	C	262	GLU	2.2
1	B	103	GLY	2.1
1	A	317	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

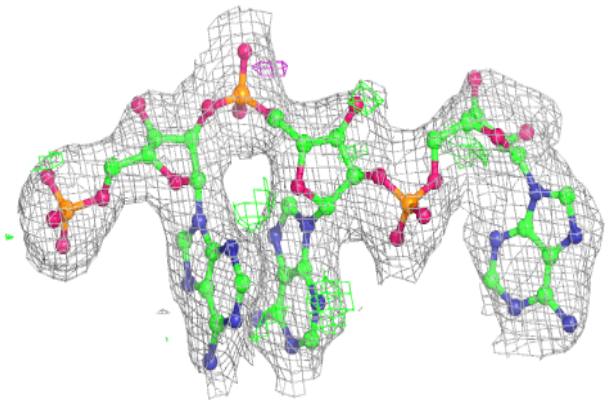
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	25A	B	401	67/67	0.95	0.18	29,55,74,87	0
2	25A	A	401	67/67	0.96	0.19	36,54,73,85	0
2	25A	C	401	67/67	0.96	0.19	31,55,71,91	0
2	25A	D	401	67/67	0.96	0.19	37,55,73,88	0

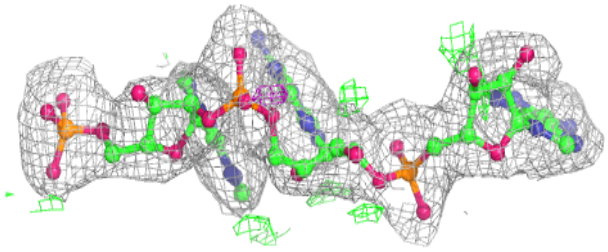
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

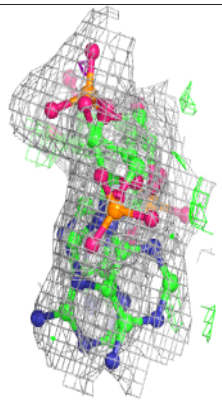
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 25A B 401:

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

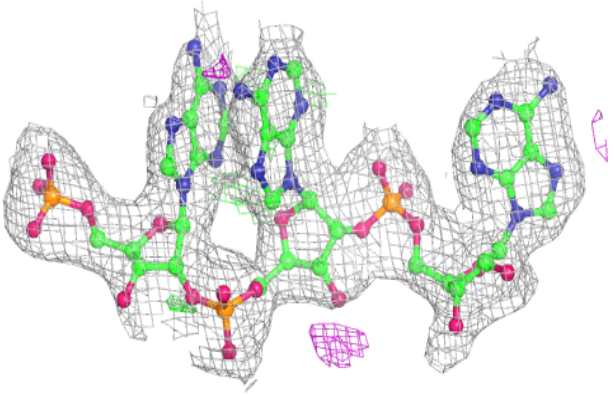


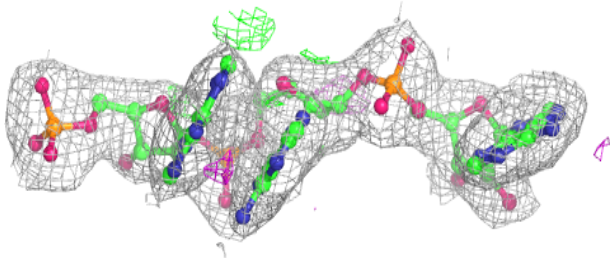


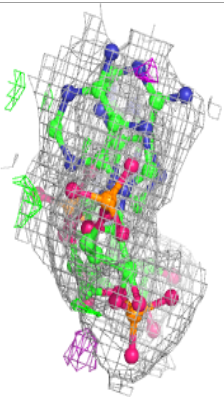


Electron density around 25A A 401:

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

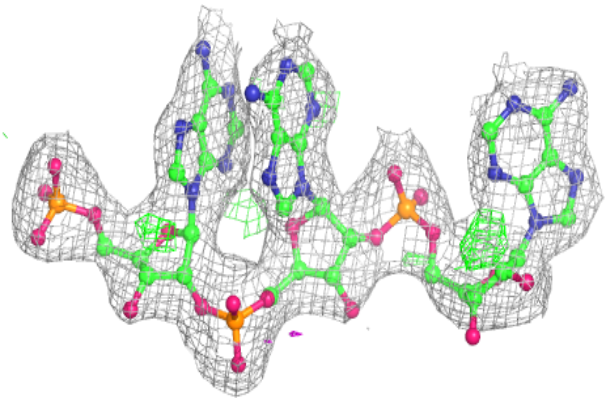


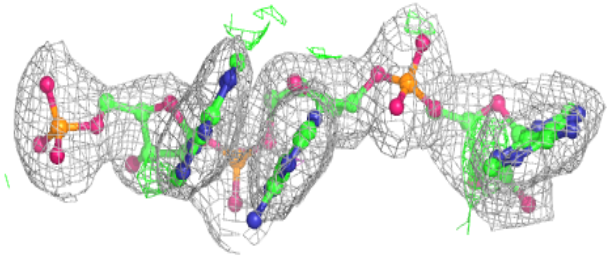


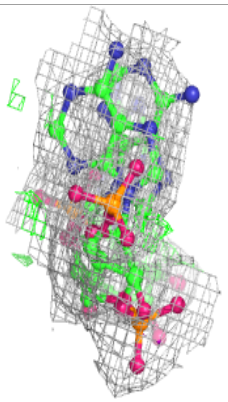


Electron density around 25A C 401:

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

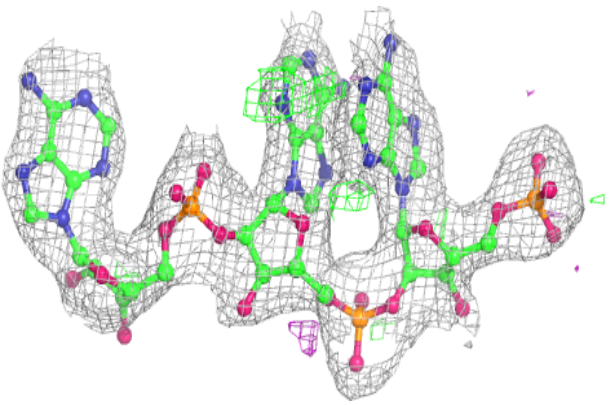


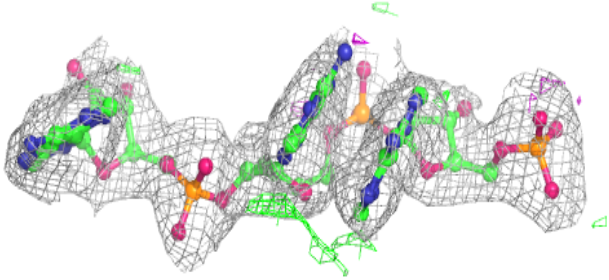


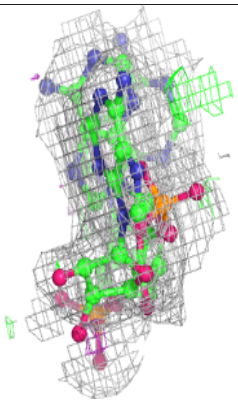


Electron density around 25A D 401:

$2mF_o$-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.