Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 10:04 am GMT

PDB ID	:	5AO1
Title	:	Crystal structure of human SAMHD1 (amino acid residues 115-583) bound to ddGTP
Authors	:	Schwefel, D.; Taylor, I.A.
Deposited on	:	2015-09-09
Resolution	:	2.54 Å(reported)

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

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

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

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

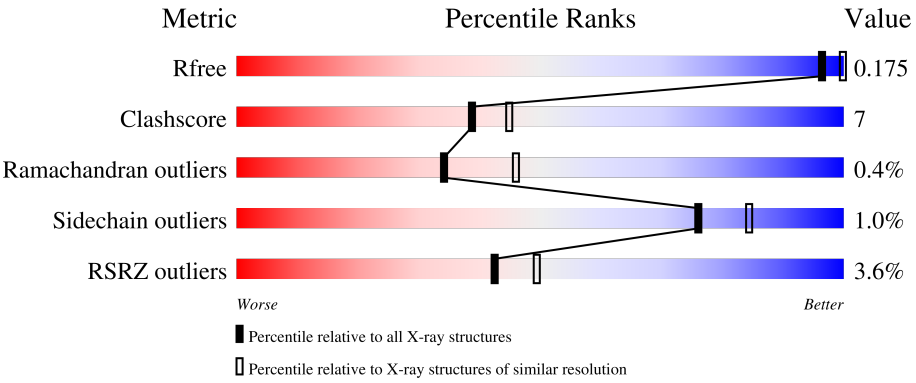
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	491	4% 78% 15% 7%
1	B	491	3% 73% 16% • 10%
1	C	491	3% 77% 16% 7%
1	D	491	3% 77% 12% • 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14581 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 DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	1	0
			3601	2311	613	657	20			
1	B	443	Total	C	N	O	S	0	0	0
			3475	2224	592	640	19			
1	C	457	Total	C	N	O	S	0	0	0
			3613	2317	612	664	20			
1	D	442	Total	C	N	O	S	0	1	0
			3454	2216	591	627	20			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	MET	-	expression tag	UNP Q9Y3Z3
A	94	ALA	-	expression tag	UNP Q9Y3Z3
A	95	SER	-	expression tag	UNP Q9Y3Z3
A	96	TRP	-	expression tag	UNP Q9Y3Z3
A	97	SER	-	expression tag	UNP Q9Y3Z3
A	98	HIS	-	expression tag	UNP Q9Y3Z3
A	99	PRO	-	expression tag	UNP Q9Y3Z3
A	100	GLN	-	expression tag	UNP Q9Y3Z3
A	101	PHE	-	expression tag	UNP Q9Y3Z3
A	102	GLU	-	expression tag	UNP Q9Y3Z3
A	103	LYS	-	expression tag	UNP Q9Y3Z3
A	104	GLY	-	expression tag	UNP Q9Y3Z3
A	105	ALA	-	expression tag	UNP Q9Y3Z3
A	106	LEU	-	expression tag	UNP Q9Y3Z3
A	107	GLU	-	expression tag	UNP Q9Y3Z3
A	108	VAL	-	expression tag	UNP Q9Y3Z3
A	109	LEU	-	expression tag	UNP Q9Y3Z3
A	110	PHE	-	expression tag	UNP Q9Y3Z3
A	111	GLN	-	expression tag	UNP Q9Y3Z3
A	112	GLY	-	expression tag	UNP Q9Y3Z3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	PRO	-	expression tag	UNP Q9Y3Z3
A	114	GLY	-	expression tag	UNP Q9Y3Z3
B	93	MET	-	expression tag	UNP Q9Y3Z3
B	94	ALA	-	expression tag	UNP Q9Y3Z3
B	95	SER	-	expression tag	UNP Q9Y3Z3
B	96	TRP	-	expression tag	UNP Q9Y3Z3
B	97	SER	-	expression tag	UNP Q9Y3Z3
B	98	HIS	-	expression tag	UNP Q9Y3Z3
B	99	PRO	-	expression tag	UNP Q9Y3Z3
B	100	GLN	-	expression tag	UNP Q9Y3Z3
B	101	PHE	-	expression tag	UNP Q9Y3Z3
B	102	GLU	-	expression tag	UNP Q9Y3Z3
B	103	LYS	-	expression tag	UNP Q9Y3Z3
B	104	GLY	-	expression tag	UNP Q9Y3Z3
B	105	ALA	-	expression tag	UNP Q9Y3Z3
B	106	LEU	-	expression tag	UNP Q9Y3Z3
B	107	GLU	-	expression tag	UNP Q9Y3Z3
B	108	VAL	-	expression tag	UNP Q9Y3Z3
B	109	LEU	-	expression tag	UNP Q9Y3Z3
B	110	PHE	-	expression tag	UNP Q9Y3Z3
B	111	GLN	-	expression tag	UNP Q9Y3Z3
B	112	GLY	-	expression tag	UNP Q9Y3Z3
B	113	PRO	-	expression tag	UNP Q9Y3Z3
B	114	GLY	-	expression tag	UNP Q9Y3Z3
C	93	MET	-	expression tag	UNP Q9Y3Z3
C	94	ALA	-	expression tag	UNP Q9Y3Z3
C	95	SER	-	expression tag	UNP Q9Y3Z3
C	96	TRP	-	expression tag	UNP Q9Y3Z3
C	97	SER	-	expression tag	UNP Q9Y3Z3
C	98	HIS	-	expression tag	UNP Q9Y3Z3
C	99	PRO	-	expression tag	UNP Q9Y3Z3
C	100	GLN	-	expression tag	UNP Q9Y3Z3
C	101	PHE	-	expression tag	UNP Q9Y3Z3
C	102	GLU	-	expression tag	UNP Q9Y3Z3
C	103	LYS	-	expression tag	UNP Q9Y3Z3
C	104	GLY	-	expression tag	UNP Q9Y3Z3
C	105	ALA	-	expression tag	UNP Q9Y3Z3
C	106	LEU	-	expression tag	UNP Q9Y3Z3
C	107	GLU	-	expression tag	UNP Q9Y3Z3
C	108	VAL	-	expression tag	UNP Q9Y3Z3
C	109	LEU	-	expression tag	UNP Q9Y3Z3
C	110	PHE	-	expression tag	UNP Q9Y3Z3

Continued on next page...

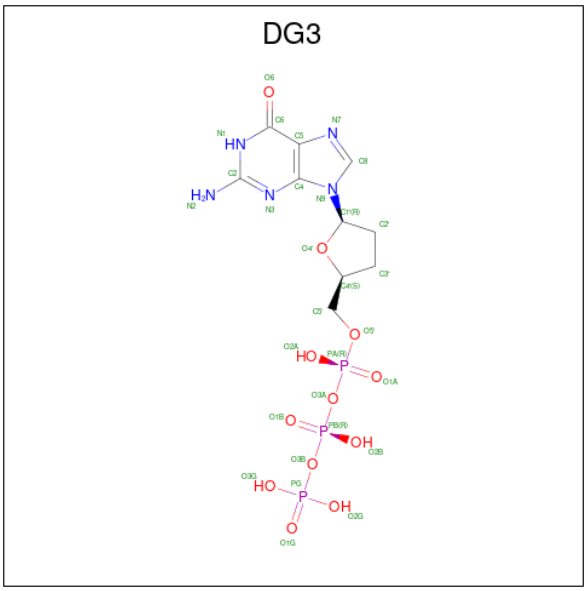
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	111	GLN	-	expression tag	UNP Q9Y3Z3
C	112	GLY	-	expression tag	UNP Q9Y3Z3
C	113	PRO	-	expression tag	UNP Q9Y3Z3
C	114	GLY	-	expression tag	UNP Q9Y3Z3
D	93	MET	-	expression tag	UNP Q9Y3Z3
D	94	ALA	-	expression tag	UNP Q9Y3Z3
D	95	SER	-	expression tag	UNP Q9Y3Z3
D	96	TRP	-	expression tag	UNP Q9Y3Z3
D	97	SER	-	expression tag	UNP Q9Y3Z3
D	98	HIS	-	expression tag	UNP Q9Y3Z3
D	99	PRO	-	expression tag	UNP Q9Y3Z3
D	100	GLN	-	expression tag	UNP Q9Y3Z3
D	101	PHE	-	expression tag	UNP Q9Y3Z3
D	102	GLU	-	expression tag	UNP Q9Y3Z3
D	103	LYS	-	expression tag	UNP Q9Y3Z3
D	104	GLY	-	expression tag	UNP Q9Y3Z3
D	105	ALA	-	expression tag	UNP Q9Y3Z3
D	106	LEU	-	expression tag	UNP Q9Y3Z3
D	107	GLU	-	expression tag	UNP Q9Y3Z3
D	108	VAL	-	expression tag	UNP Q9Y3Z3
D	109	LEU	-	expression tag	UNP Q9Y3Z3
D	110	PHE	-	expression tag	UNP Q9Y3Z3
D	111	GLN	-	expression tag	UNP Q9Y3Z3
D	112	GLY	-	expression tag	UNP Q9Y3Z3
D	113	PRO	-	expression tag	UNP Q9Y3Z3
D	114	GLY	-	expression tag	UNP Q9Y3Z3

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

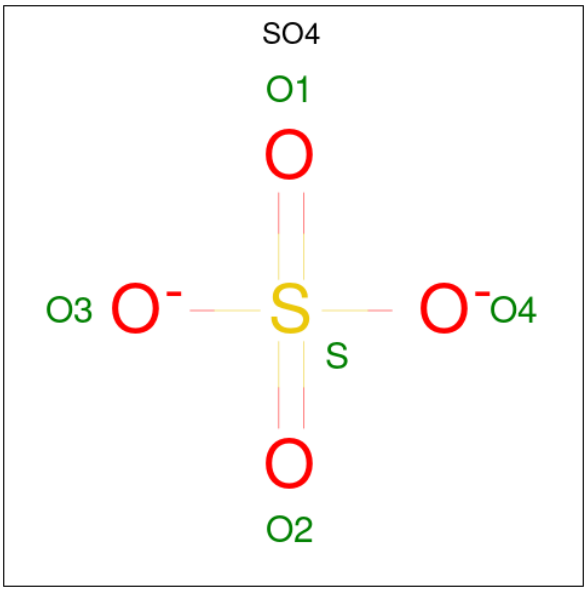
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mg 2 2	0	0
5	D	2	Total Mg 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	55	Total O 55 55	0	0
6	B	33	Total O 33 33	0	0
6	C	40	Total O 40 40	0	0

Continued on next page...

Continued from previous page...

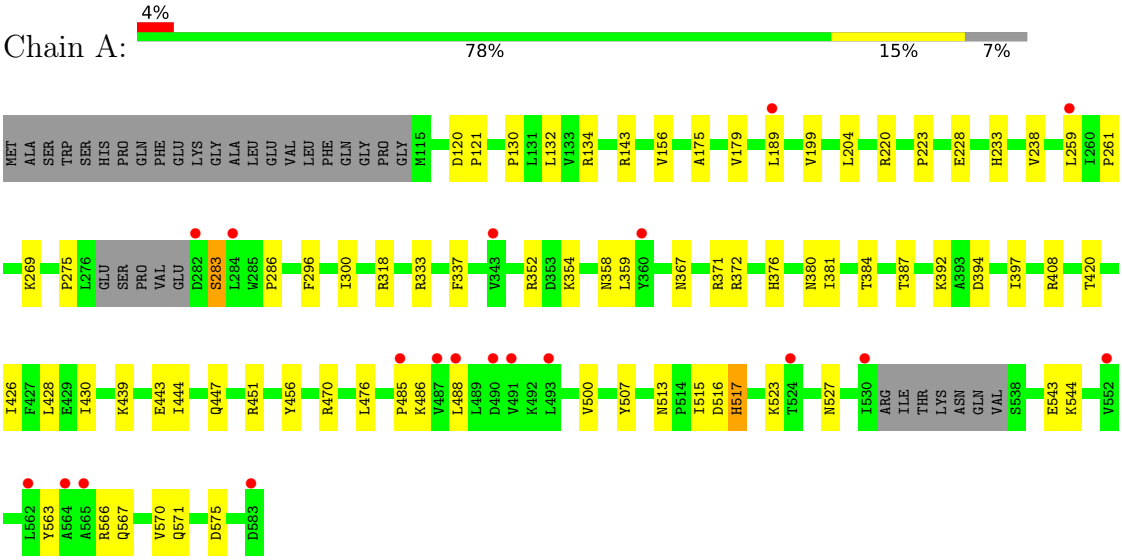
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	42	Total	O	0	0
			42	42		

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.

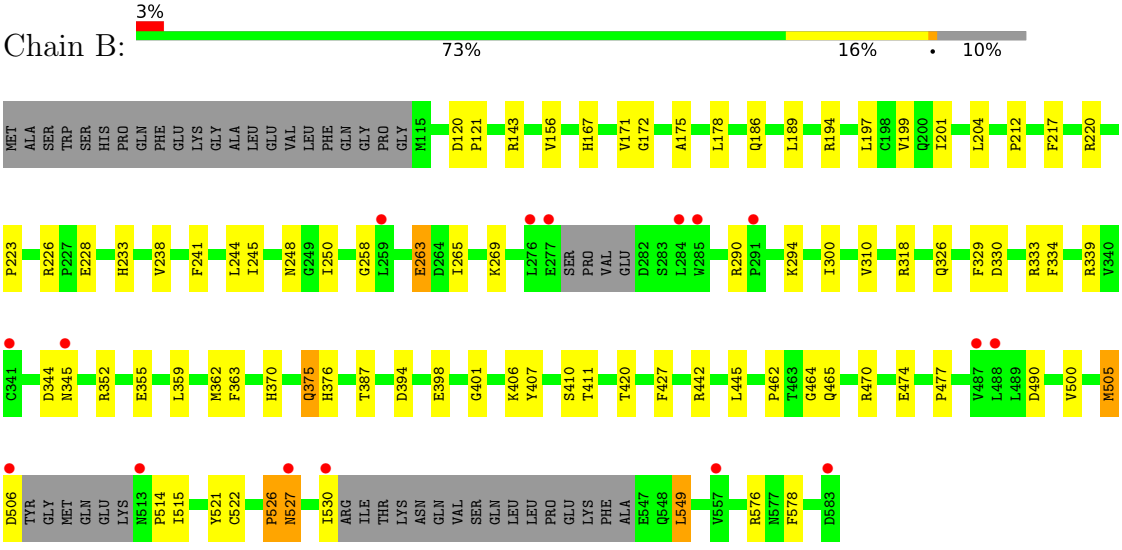
• Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

Chain A:



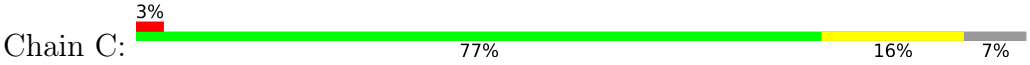
• Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

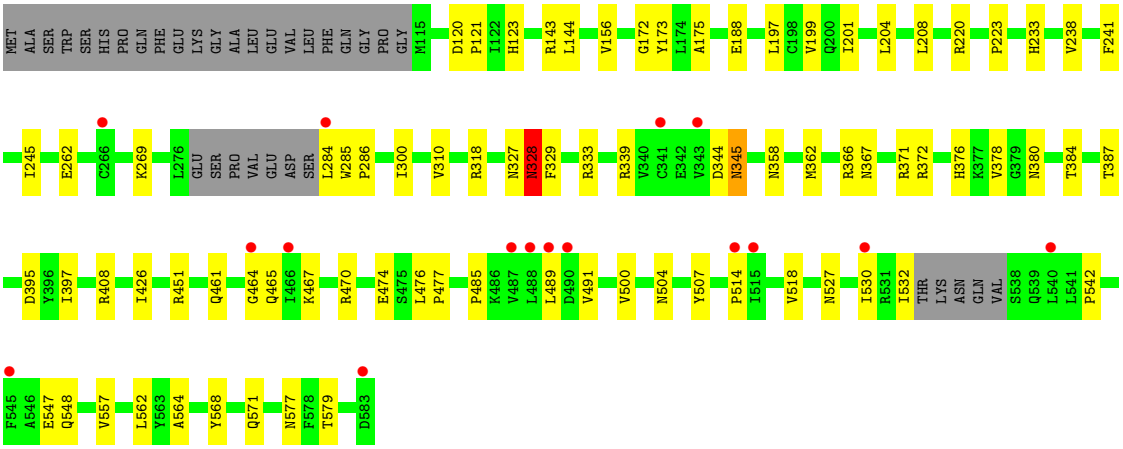
Chain B:



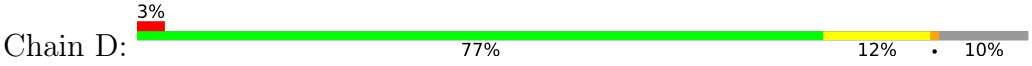
• Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

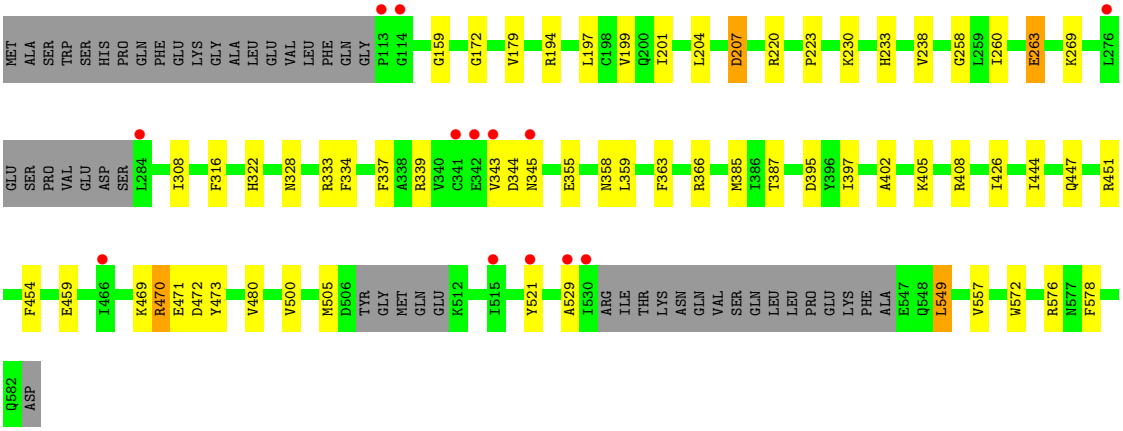
Chain C:





• Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.12Å 187.36Å 81.37Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	49.23 – 2.54 49.23 – 2.54	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.23-2.54) 96.7 (49.23-2.54)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.171 , 0.220 0.176 , 0.175	Depositor DCC
R_{free} test set	3309 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14581	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DG3, SO4, FE

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	0.50	0/3692	0.72	3/5002 (0.1%)
1	B	0.54	0/3558	0.70	1/4827 (0.0%)
1	C	0.46	0/3701	0.65	1/5017 (0.0%)
1	D	0.57	2/3542 (0.1%)	0.71	3/4798 (0.1%)
All	All	0.52	2/14493 (0.0%)	0.70	8/19644 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	263	GLU	CB-CG	14.17	1.79	1.52
1	D	263	GLU	CG-CD	5.45	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	488	LEU	CA-CB-CG	9.61	137.39	115.30
1	A	488	LEU	CB-CG-CD1	8.75	125.88	111.00
1	A	543	GLU	C-N-CA	5.96	136.59	121.70
1	D	470	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	263	GLU	OE1-CD-OE2	-5.87	116.26	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	207	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	344	ASP	C-N-CA	5.66	135.86	121.70
1	D	207	ASP	CB-CG-OD1	-5.59	113.27	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	PRO	Peptide
1	A	486	LYS	Peptide
1	A	527	ASN	Peptide
1	C	328	ASN	Sidechain

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	3601	0	3425	44	0
1	B	3475	0	3271	58	0
1	C	3613	0	3427	56	0
1	D	3454	0	3266	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	30	0	12	2	0
3	B	90	0	36	3	0
3	C	30	0	12	1	0
3	D	90	0	36	8	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	D	10	0	0	0	0
5	B	2	0	0	0	0
5	D	2	0	0	0	0
6	A	55	0	0	1	0
6	B	33	0	0	2	0
6	C	40	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	42	0	0	5	0
All	All	14581	0	13485	209	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 7.

All (209) 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:D:263:GLU:CB	1:D:263:GLU:CG	1.79	1.52
1:B:194:ARG:NH2	1:B:263:GLU:OE1	1.92	1.01
1:D:469:LYS:HG3	1:D:471:GLU:HG2	1.48	0.95
1:B:290:ARG:HD2	1:B:294:LYS:HD3	1.59	0.83
1:C:328:ASN:HD22	1:C:328:ASN:N	1.76	0.81
1:A:372:ARG:NH1	4:A:1586:SO4:O3	2.14	0.80
1:B:233:HIS:NE2	3:B:1587:DG3:O1G	2.16	0.79
1:D:220:ARG:NH2	1:D:500:VAL:O	2.16	0.77
1:D:451:ARG:HH21	3:D:1583:DG3:H5'1	1.48	0.77
1:C:233:HIS:NE2	3:C:1585:DG3:O2G	2.19	0.76
1:D:576:ARG:HH11	1:D:578:PHE:HZ	1.33	0.76
1:B:344:ASP:O	1:B:345:ASN:HB3	1.87	0.74
1:A:233:HIS:NE2	3:A:1585:DG3:O2G	2.22	0.73
1:C:371:ARG:NH2	1:C:547:GLU:OE2	2.23	0.71
1:C:485:PRO:HA	1:C:571:GLN:HG3	1.74	0.70
1:D:344:ASP:O	1:D:345:ASN:HB3	1.92	0.70
1:A:352:ARG:HH11	1:A:352:ARG:HG2	1.58	0.68
1:C:557:VAL:HA	1:C:562:LEU:HD11	1.77	0.67
1:D:469:LYS:CG	1:D:471:GLU:HG2	2.23	0.67
1:B:220:ARG:NH2	1:B:500:VAL:O	2.28	0.67
1:B:370:HIS:O	1:B:375:GLN:HB2	1.94	0.66
1:C:345:ASN:HD22	1:C:345:ASN:N	1.93	0.66
1:B:326:GLN:OE1	1:D:328:ASN:ND2	2.28	0.66
1:D:333:ARG:NH2	1:D:355:GLU:HA	2.11	0.66
1:B:352:ARG:HG3	1:B:521:TYR:CZ	2.31	0.65
1:A:571:GLN:NE2	1:A:575:ASP:OD1	2.30	0.65
1:C:451:ARG:HH21	3:D:1587:DG3:H5'1	1.62	0.64
1:A:476:LEU:HB2	1:A:500:VAL:HG11	1.81	0.63
1:D:230:LYS:NZ	6:D:2020:HOH:O	2.31	0.63
1:D:469:LYS:HG3	1:D:471:GLU:CG	2.27	0.63
1:C:328:ASN:N	1:C:328:ASN:ND2	2.47	0.62
1:B:143:ARG:HD3	6:B:2002:HOH:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HH21	3:B:1588:DG3:H5'1	1.65	0.62
1:D:233:HIS:NE2	3:D:1586:DG3:O2G	2.33	0.62
1:A:120:ASP:OD1	1:A:318:ARG:NH2	2.33	0.61
1:B:330:ASP:OD2	1:B:333:ARG:HG3	2.01	0.61
1:D:260:ILE:HG21	1:D:263:GLU:OE2	2.00	0.61
1:A:476:LEU:CB	1:A:500:VAL:HG11	2.31	0.60
1:C:366:ARG:HH11	1:C:366:ARG:HG2	1.66	0.60
1:A:238:VAL:HG13	1:A:269:LYS:HD3	1.84	0.59
1:B:339:ARG:HD3	1:B:521:TYR:CE2	2.37	0.59
1:C:476:LEU:CB	1:C:500:VAL:HG11	2.32	0.59
1:D:316:PHE:CZ	1:D:366:ARG:HB2	2.38	0.59
1:C:241:PHE:CZ	1:C:245:ILE:HD11	2.39	0.58
1:C:333:ARG:NH2	1:C:358:ASN:HB2	2.18	0.58
1:D:333:ARG:HH22	1:D:355:GLU:HA	1.67	0.58
1:C:220:ARG:NH2	1:C:500:VAL:O	2.36	0.58
1:D:402:ALA:O	1:D:405:LYS:HG3	2.03	0.58
1:B:245:ILE:HG23	1:B:250:ILE:HB	1.86	0.58
1:B:462:PRO:HA	1:B:578:PHE:CD1	2.39	0.58
1:C:339:ARG:NH2	1:C:527:ASN:OD1	2.34	0.57
1:D:238:VAL:HG13	1:D:269:LYS:HD3	1.86	0.57
1:C:489:LEU:HD13	1:C:491:VAL:O	2.05	0.57
1:D:263:GLU:CB	1:D:263:GLU:CD	2.72	0.57
1:C:564:ALA:HB1	1:C:568:TYR:HE2	1.69	0.56
1:B:223:PRO:HG3	1:B:470:ARG:HG2	1.87	0.56
1:A:470:ARG:HD3	1:A:507:TYR:CZ	2.41	0.56
1:B:505:MET:SD	1:B:505:MET:N	2.78	0.56
1:A:470:ARG:HD2	6:A:2023:HOH:O	2.04	0.56
1:B:442:ARG:NH2	4:B:1589:SO4:O3	2.39	0.56
1:B:167:HIS:HA	1:B:318:ARG:HH11	1.71	0.56
1:B:238:VAL:HG13	1:B:269:LYS:HD3	1.88	0.55
1:B:228:GLU:CD	1:B:228:GLU:H	2.09	0.54
1:A:156:VAL:HG11	1:A:376:HIS:CE1	2.42	0.54
1:A:513:ASN:OD1	1:A:515:ILE:HG22	2.07	0.54
1:B:220:ARG:HG2	1:B:387:THR:HG21	1.89	0.54
1:C:395:ASP:OD1	1:C:408:ARG:NH1	2.41	0.54
1:D:223:PRO:HG3	1:D:470:ARG:HG2	1.90	0.54
1:C:470:ARG:HD3	1:C:507:TYR:CZ	2.43	0.53
1:D:576:ARG:NH1	1:D:578:PHE:HZ	2.03	0.53
1:C:367:ASN:ND2	1:C:542:PRO:HB3	2.24	0.53
1:D:469:LYS:CD	1:D:470:ARG:N	2.72	0.53
1:B:194:ARG:HD2	1:B:258:GLY:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ASN:N	1:C:345:ASN:ND2	2.56	0.52
1:D:444:ILE:O	1:D:447:GLN:HB2	2.09	0.52
1:C:397:ILE:HG21	1:C:426:ILE:HD11	1.93	0.51
1:B:330:ASP:CG	1:B:333:ARG:HG3	2.31	0.51
1:B:197:LEU:O	1:B:201:ILE:HG13	2.10	0.51
1:D:223:PRO:CG	1:D:470:ARG:HG2	2.41	0.51
1:C:238:VAL:HG13	1:C:269:LYS:HD3	1.93	0.51
1:D:451:ARG:NH2	3:D:1583:DG3:H5'1	2.21	0.51
1:C:476:LEU:HB3	1:C:500:VAL:HG11	1.93	0.50
1:B:401:GLY:HA3	1:B:407:TYR:CE1	2.47	0.50
1:D:159:GLY:O	1:D:322:HIS:HB3	2.12	0.50
1:D:339:ARG:HD3	1:D:521:TYR:CE1	2.47	0.50
1:A:516:ASP:O	1:A:517:HIS:ND1	2.39	0.50
1:D:395:ASP:OD1	1:D:408:ARG:NH1	2.45	0.50
1:C:366:ARG:HG2	1:C:366:ARG:NH1	2.26	0.50
1:A:397:ILE:HG21	1:A:426:ILE:HD11	1.94	0.49
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.93	0.49
1:B:334:PHE:CE2	1:B:359:LEU:HD21	2.47	0.49
1:C:476:LEU:HB2	1:C:500:VAL:HG11	1.93	0.49
1:A:439:LYS:O	1:A:443:GLU:HG2	2.12	0.49
1:A:392:LYS:NZ	1:A:444:ILE:HD11	2.27	0.49
1:B:156:VAL:O	3:B:1584:DG3:H8	2.12	0.49
1:B:156:VAL:HG11	1:B:376:HIS:CE1	2.48	0.49
1:B:370:HIS:HE1	6:B:2019:HOH:O	1.94	0.49
1:C:123:HIS:HB3	1:C:173:TYR:CE2	2.48	0.49
1:C:467:LYS:HB3	1:C:548:GLN:OE1	2.12	0.49
1:B:522:CYS:HB2	1:B:530:ILE:HD11	1.94	0.49
1:D:207:ASP:OD1	3:D:1586:DG3:O2G	2.30	0.49
1:B:398:GLU:HB3	1:B:406:LYS:HD3	1.95	0.48
1:B:339:ARG:HD3	1:B:521:TYR:CZ	2.47	0.48
1:C:223:PRO:HG3	1:C:470:ARG:HG2	1.95	0.48
1:A:352:ARG:NH2	1:A:523:LYS:HB2	2.29	0.48
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.14	0.48
1:D:343:VAL:HG22	1:D:529:ALA:HB2	1.95	0.48
1:B:576:ARG:HD3	1:B:578:PHE:CE2	2.49	0.48
1:B:363:PHE:CD2	1:B:514:PRO:HG2	2.49	0.48
1:C:380:ASN:O	1:C:384:THR:HG23	2.14	0.48
1:A:397:ILE:HD11	1:A:430:ILE:HG12	1.96	0.47
1:B:244:LEU:O	1:B:248:ASN:ND2	2.42	0.47
1:C:465:GLN:HE22	1:C:577:ASN:HB2	1.80	0.47
1:C:300:ILE:O	1:C:310:VAL:HG22	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ARG:HD2	1:D:258:GLY:O	2.16	0.46
1:D:557:VAL:HG11	6:D:2034:HOH:O	2.14	0.46
1:A:380:ASN:O	1:A:384:THR:HG23	2.14	0.46
1:B:172:GLY:HA3	1:B:204:LEU:HD13	1.98	0.46
1:B:576:ARG:HD3	1:B:578:PHE:CZ	2.50	0.46
1:A:394:ASP:O	1:A:408:ARG:CG	2.63	0.46
1:D:233:HIS:CD2	3:D:1586:DG3:O2G	2.68	0.46
1:A:132:LEU:HB3	1:A:204:LEU:HD11	1.98	0.46
1:B:339:ARG:HB2	1:B:521:TYR:CE1	2.51	0.46
1:C:378:VAL:HG11	3:D:1587:DG3:H5'2	1.98	0.46
1:A:130:PRO:O	1:A:134:ARG:HG2	2.16	0.46
1:A:220:ARG:HG2	1:A:387:THR:HG21	1.98	0.46
1:B:474:GLU:O	1:B:477:PRO:HD2	2.16	0.46
1:D:333:ARG:HH21	1:D:358:ASN:HB2	1.80	0.46
1:B:171:VAL:HG13	1:B:310:VAL:HG23	1.98	0.45
1:B:226:ARG:NH1	1:B:411:THR:HA	2.31	0.45
1:C:329:PHE:HB2	1:C:362:MET:HA	1.98	0.45
1:C:474:GLU:O	1:C:477:PRO:HD2	2.16	0.45
1:D:179:VAL:HG11	1:D:199:VAL:HG21	1.98	0.45
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.83	0.45
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.16	0.45
1:C:461:GLN:O	1:C:579:THR:HG23	2.17	0.45
1:C:329:PHE:CD1	1:C:362:MET:HB2	2.51	0.45
1:D:334:PHE:CE2	1:D:359:LEU:HD21	2.52	0.45
1:A:566:ARG:O	1:A:570:VAL:HG23	2.17	0.44
1:C:318:ARG:NH1	6:C:2023:HOH:O	2.34	0.44
1:D:470:ARG:HG3	1:D:473:TYR:CE2	2.52	0.44
1:B:526:PRO:O	1:B:527:ASN:OD1	2.36	0.44
1:D:472:ASP:OD2	6:D:2035:HOH:O	2.20	0.44
1:B:505:MET:HE2	1:B:549:LEU:HD23	1.99	0.44
1:A:515:ILE:HD12	1:A:515:ILE:HA	1.92	0.44
1:A:563:TYR:O	1:A:567:GLN:HG2	2.18	0.44
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.99	0.44
1:D:233:HIS:HE1	6:D:2012:HOH:O	1.99	0.44
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.18	0.44
1:D:459:GLU:OE1	1:D:549:LEU:HD21	2.18	0.44
1:A:337:PHE:CD1	1:A:352:ARG:HD2	2.52	0.44
1:A:259:LEU:O	1:A:261:PRO:HD3	2.18	0.43
1:A:443:GLU:O	1:A:447[B]:GLN:HG3	2.17	0.43
1:C:467:LYS:HB3	1:C:548:GLN:CD	2.38	0.43
1:C:514:PRO:O	1:C:518:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:PHE:CE2	1:B:445:LEU:HD22	2.53	0.43
1:C:285:TRP:HA	1:C:286:PRO:HD3	1.88	0.43
1:D:345:ASN:O	1:D:345:ASN:OD1	2.35	0.43
1:C:143:ARG:HD3	6:C:2004:HOH:O	2.19	0.43
1:C:156:VAL:HG11	1:C:376:HIS:CE1	2.54	0.43
1:D:197:LEU:O	1:D:201:ILE:HG13	2.18	0.43
1:B:265:ILE:CG2	1:B:269:LYS:HE3	2.49	0.43
1:D:385:MET:HG2	1:D:454:PHE:CE2	2.54	0.43
1:D:172:GLY:HA3	1:D:204:LEU:HD13	2.00	0.42
1:C:241:PHE:CE2	1:C:245:ILE:HD11	2.54	0.42
1:B:359:LEU:HA	1:B:359:LEU:HD23	1.69	0.42
1:C:144:LEU:HD11	1:C:208:LEU:HD23	2.01	0.42
1:C:220:ARG:HG2	1:C:387:THR:HG21	2.02	0.42
1:B:120:ASP:OD2	1:B:318:ARG:NH2	2.53	0.42
1:B:401:GLY:HA3	1:B:407:TYR:HE1	1.85	0.42
1:A:189:LEU:HD22	1:A:296:PHE:CE1	2.55	0.42
1:A:476:LEU:HB3	1:A:500:VAL:HG11	2.02	0.42
1:B:143:ARG:HD2	1:B:420:THR:HA	2.02	0.42
1:D:337:PHE:N	1:D:337:PHE:CD1	2.86	0.42
1:D:359:LEU:HD23	1:D:359:LEU:HA	1.83	0.42
1:A:179:VAL:HG13	1:A:300:ILE:HD13	2.01	0.41
1:B:178:LEU:HD23	1:B:300:ILE:HG12	2.01	0.41
1:C:156:VAL:O	3:D:1587:DG3:H8	2.20	0.41
1:D:397:ILE:HG21	1:D:426:ILE:HD11	2.02	0.41
1:C:284:LEU:HD23	1:C:284:LEU:HA	1.86	0.41
1:A:428:LEU:HD23	1:A:428:LEU:HA	1.89	0.41
1:D:308:ILE:HD11	1:D:363:PHE:HZ	1.86	0.41
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.01	0.41
1:B:333:ARG:NH2	1:B:355:GLU:OE2	2.53	0.41
1:B:212:PRO:HD2	1:B:217:PHE:CD1	2.55	0.41
1:C:188:GLU:H	1:C:188:GLU:CD	2.24	0.41
1:B:329:PHE:CD1	1:B:362:MET:HB2	2.55	0.41
1:C:172:GLY:HA3	1:C:204:LEU:HG	2.03	0.41
1:C:327:ASN:C	1:C:328:ASN:HD22	2.22	0.41
1:D:220:ARG:HG2	1:D:387:THR:HG21	2.03	0.41
1:B:186:GLN:HB2	1:B:189:LEU:HD12	2.03	0.41
1:B:352:ARG:HG3	1:B:521:TYR:OH	2.21	0.41
1:B:394:ASP:OD2	1:B:410:SER:OG	2.36	0.41
1:C:504:ASN:OD1	1:C:548:GLN:HG3	2.21	0.41
1:C:530:ILE:O	1:C:532:ILE:HG23	2.20	0.41
1:A:143:ARG:HD2	1:A:420:THR:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PRO:HB3	1:A:286:PRO:HB2	2.03	0.40
1:A:381:ILE:HD11	1:A:456:TYR:HB2	2.03	0.40
1:C:197:LEU:O	1:C:201:ILE:HG13	2.21	0.40
1:D:469:LYS:CD	1:D:470:ARG:H	2.34	0.40
1:D:480:VAL:HG22	1:D:572:TRP:CD2	2.57	0.40
1:C:372:ARG:NE	6:C:2028:HOH:O	2.46	0.40
1:D:470:ARG:HD2	6:D:2016:HOH:O	2.19	0.40
1:B:241:PHE:CZ	1:B:245:ILE:HD11	2.55	0.40
1:A:223:PRO:HG3	1:A:470:ARG:HG2	2.02	0.40
1:A:333:ARG:NH2	1:A:358:ASN:HB2	2.37	0.40
1:A:233:HIS:CD2	3:A:1585:DG3:O2G	2.74	0.40
1:A:367:ASN:O	1:A:371:ARG:HG2	2.21	0.40
1:D:204:LEU:HD12	1:D:204:LEU:HA	1.96	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	452/491 (92%)	441 (98%)	8 (2%)	3 (1%)	22	30
1	B	435/491 (89%)	422 (97%)	10 (2%)	3 (1%)	22	30
1	C	451/491 (92%)	443 (98%)	7 (2%)	1 (0%)	47	60
1	D	435/491 (89%)	428 (98%)	7 (2%)	0	100	100
All	All	1773/1964 (90%)	1734 (98%)	32 (2%)	7 (0%)	34	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	B	465	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	544	LYS
1	B	464	GLY
1	B	526	PRO
1	C	464	GLY
1	A	517	HIS

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	370/434 (85%)	367 (99%)	3 (1%)	81	88
1	B	356/434 (82%)	349 (98%)	7 (2%)	55	70
1	C	372/434 (86%)	369 (99%)	3 (1%)	81	88
1	D	351/434 (81%)	348 (99%)	3 (1%)	78	86
All	All	1449/1736 (84%)	1433 (99%)	16 (1%)	76	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	GLU
1	A	283	SER
1	A	354	LYS
1	B	375	GLN
1	B	490	ASP
1	B	505	MET
1	B	506	ASP
1	B	515	ILE
1	B	527	ASN
1	B	549	LEU
1	C	262	GLU
1	C	328	ASN
1	C	345	ASN
1	D	505[A]	MET
1	D	505[B]	MET
1	D	549	LEU

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

Mol	Chain	Res	Type
1	B	375	GLN
1	C	345	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)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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	DG3	D	1587	5	25,32,32	0.92	1 (4%)	28,50,50	1.33	3 (10%)
3	DG3	D	1583	5	25,32,32	0.92	1 (4%)	28,50,50	1.59	6 (21%)
4	SO4	D	1588	-	4,4,4	0.15	0	6,6,6	0.16	0
3	DG3	C	1585	2	25,32,32	0.83	1 (4%)	28,50,50	1.63	8 (28%)
3	DG3	B	1584	5	25,32,32	0.98	1 (4%)	28,50,50	1.49	5 (17%)
4	SO4	B	1589	-	4,4,4	0.15	0	6,6,6	0.08	0
3	DG3	A	1585	2	25,32,32	0.90	1 (4%)	28,50,50	1.43	4 (14%)
3	DG3	B	1588	5	25,32,32	0.87	1 (4%)	28,50,50	1.66	6 (21%)
3	DG3	B	1587	2	25,32,32	0.85	1 (4%)	28,50,50	1.44	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	1586	-	4,4,4	0.18	0	6,6,6	0.12	0
4	SO4	D	1589	-	4,4,4	0.16	0	6,6,6	0.45	0
3	DG3	D	1586	2	25,32,32	0.87	0	28,50,50	1.50	6 (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
3	DG3	D	1587	5	-	3/18/31/31	0/3/3/3
3	DG3	D	1583	5	-	7/18/31/31	0/3/3/3
3	DG3	C	1585	2	-	2/18/31/31	0/3/3/3
3	DG3	B	1584	5	-	5/18/31/31	0/3/3/3
3	DG3	A	1585	2	-	3/18/31/31	0/3/3/3
3	DG3	B	1588	5	-	5/18/31/31	0/3/3/3
3	DG3	B	1587	2	-	8/18/31/31	0/3/3/3
3	DG3	D	1586	2	-	5/18/31/31	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1584	DG3	C6-N1	-3.05	1.33	1.37
3	D	1587	DG3	C6-N1	-2.62	1.34	1.37
3	A	1585	DG3	C6-N1	-2.57	1.34	1.37
3	D	1583	DG3	C6-N1	-2.38	1.34	1.37
3	C	1585	DG3	C6-N1	-2.09	1.34	1.37
3	B	1587	DG3	C5-C4	2.06	1.48	1.43
3	B	1588	DG3	C6-N1	-2.05	1.34	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1588	DG3	O4'-C4'-C5'	-3.82	103.24	109.52
3	C	1585	DG3	O4'-C4'-C5'	-3.11	104.40	109.52
3	D	1583	DG3	PB-O3B-PG	-2.97	122.64	132.83
3	A	1585	DG3	PB-O3B-PG	-2.96	122.66	132.83
3	D	1583	DG3	C8-N7-C5	2.93	108.57	102.99
3	D	1583	DG3	C3'-C2'-C1'	2.76	105.97	102.78
3	A	1585	DG3	C8-N7-C5	2.70	108.13	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1584	DG3	PA-O3A-PB	-2.65	123.72	132.83
3	C	1585	DG3	PB-O3B-PG	-2.65	123.74	132.83
3	B	1588	DG3	C8-N7-C5	2.64	108.01	102.99
3	B	1588	DG3	PA-O3A-PB	-2.60	123.89	132.83
3	B	1588	DG3	C4'-O4'-C1'	2.59	112.25	109.81
3	B	1584	DG3	C8-N7-C5	2.54	107.83	102.99
3	C	1585	DG3	C8-N7-C5	2.51	107.78	102.99
3	B	1584	DG3	C4'-O4'-C1'	-2.51	107.44	109.81
3	B	1587	DG3	PB-O3B-PG	-2.50	124.23	132.83
3	D	1586	DG3	O6-C6-C5	-2.50	119.49	124.37
3	C	1585	DG3	O6-C6-C5	-2.46	119.57	124.37
3	B	1584	DG3	C3'-C2'-C1'	2.45	105.61	102.78
3	D	1587	DG3	PB-O3B-PG	-2.45	124.43	132.83
3	D	1587	DG3	C8-N7-C5	2.43	107.62	102.99
3	D	1583	DG3	O4'-C4'-C3'	2.41	108.81	104.80
3	D	1587	DG3	C3'-C2'-C1'	2.37	105.52	102.78
3	B	1588	DG3	PB-O3B-PG	-2.37	124.68	132.83
3	C	1585	DG3	O4'-C1'-C2'	2.32	109.19	106.67
3	B	1587	DG3	O6-C6-C5	-2.31	119.86	124.37
3	B	1588	DG3	C3'-C2'-C1'	2.29	105.43	102.78
3	D	1586	DG3	C8-N7-C5	2.28	107.33	102.99
3	B	1587	DG3	C8-N7-C5	2.25	107.27	102.99
3	D	1583	DG3	O4'-C4'-C5'	-2.19	105.92	109.52
3	D	1586	DG3	PA-O3A-PB	-2.18	125.33	132.83
3	B	1584	DG3	PB-O3B-PG	-2.17	125.39	132.83
3	A	1585	DG3	C5-C6-N1	2.16	117.77	113.95
3	C	1585	DG3	C5-C6-N1	2.14	117.72	113.95
3	A	1585	DG3	O2A-PA-O1A	2.09	122.57	112.24
3	D	1583	DG3	PA-O3A-PB	-2.09	125.67	132.83
3	B	1587	DG3	PA-O3A-PB	-2.08	125.68	132.83
3	C	1585	DG3	O4'-C4'-C3'	2.06	108.23	104.80
3	D	1586	DG3	O2G-PG-O3B	-2.06	97.72	104.64
3	D	1586	DG3	O6-C6-N1	2.04	123.06	120.65
3	D	1586	DG3	C3'-C2'-C1'	2.04	105.14	102.78
3	B	1587	DG3	O4'-C1'-C2'	2.01	108.85	106.67
3	C	1585	DG3	O2A-PA-O1A	2.01	122.19	112.24
3	B	1587	DG3	O6-C6-N1	2.01	123.02	120.65

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1585	DG3	C5'-O5'-PA-O3A
3	B	1584	DG3	PB-O3B-PG-O3G
3	B	1587	DG3	C5'-O5'-PA-O3A
3	B	1587	DG3	C5'-O5'-PA-O1A
3	B	1587	DG3	C5'-O5'-PA-O2A
3	B	1588	DG3	C5'-O5'-PA-O3A
3	B	1588	DG3	C5'-O5'-PA-O2A
3	D	1583	DG3	C5'-O5'-PA-O1A
3	D	1583	DG3	C5'-O5'-PA-O2A
3	D	1583	DG3	O4'-C4'-C5'-O5'
3	D	1583	DG3	C3'-C4'-C5'-O5'
3	D	1586	DG3	C5'-O5'-PA-O1A
3	D	1587	DG3	PB-O3B-PG-O2G
3	B	1584	DG3	O4'-C4'-C5'-O5'
3	D	1586	DG3	C5'-O5'-PA-O3A
3	D	1586	DG3	PG-O3B-PB-O1B
3	A	1585	DG3	C5'-O5'-PA-O1A
3	A	1585	DG3	C5'-O5'-PA-O2A
3	B	1588	DG3	C5'-O5'-PA-O1A
3	C	1585	DG3	O4'-C4'-C5'-O5'
3	B	1587	DG3	PB-O3B-PG-O1G
3	B	1588	DG3	PG-O3B-PB-O1B
3	D	1583	DG3	PB-O3A-PA-O2A
3	B	1588	DG3	O4'-C4'-C5'-O5'
3	B	1584	DG3	PB-O3A-PA-O1A
3	B	1587	DG3	PB-O3A-PA-O1A
3	B	1587	DG3	PB-O3A-PA-O2A
3	B	1584	DG3	PB-O3B-PG-O1G
3	D	1587	DG3	PB-O3B-PG-O1G
3	B	1584	DG3	C3'-C4'-C5'-O5'
3	B	1587	DG3	C3'-C4'-C5'-O5'
3	B	1587	DG3	O4'-C4'-C5'-O5'
3	D	1586	DG3	PB-O3B-PG-O3G
3	D	1587	DG3	PB-O3B-PG-O3G
3	D	1583	DG3	C5'-O5'-PA-O3A
3	C	1585	DG3	PB-O3A-PA-O2A
3	D	1583	DG3	PA-O3A-PB-O1B
3	D	1586	DG3	PG-O3B-PB-O2B

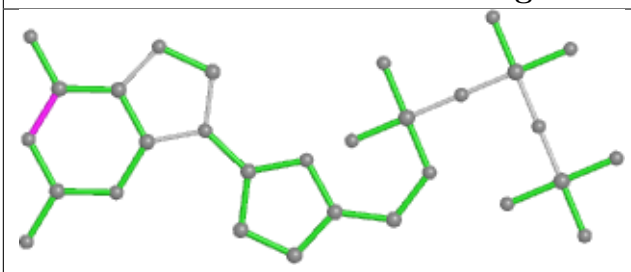
There are no ring outliers.

10 monomers are involved in 16 short contacts:

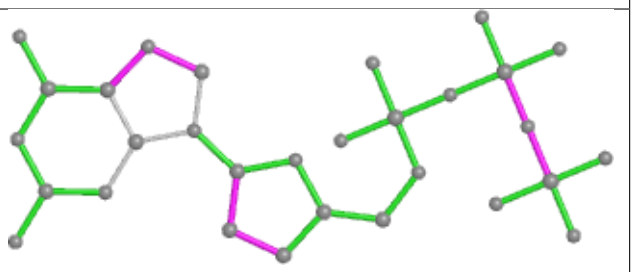
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1587	DG3	3	0
3	D	1583	DG3	2	0
3	C	1585	DG3	1	0
3	B	1584	DG3	1	0
4	B	1589	SO4	1	0
3	A	1585	DG3	2	0
3	B	1588	DG3	1	0
3	B	1587	DG3	1	0
4	A	1586	SO4	1	0
3	D	1586	DG3	3	0

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

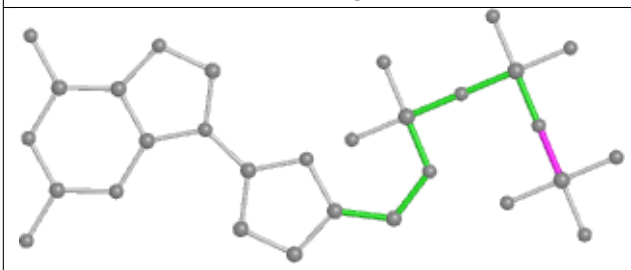
Ligand DG3 D 1587



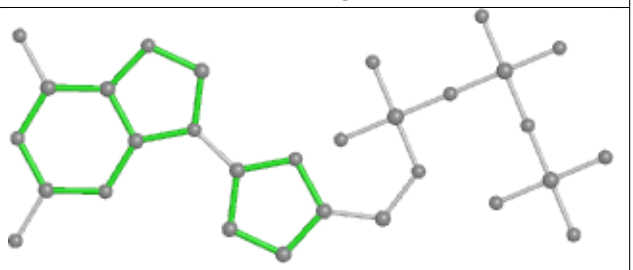
Bond lengths



Bond angles

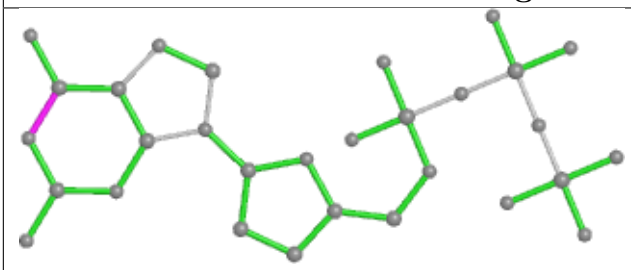


Torsions

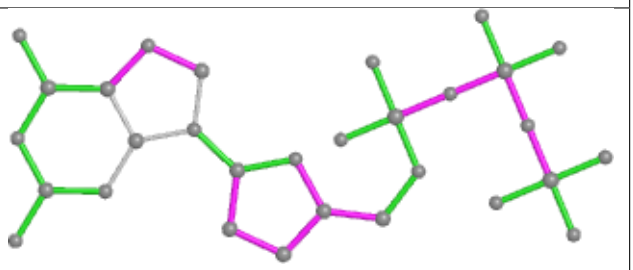


Rings

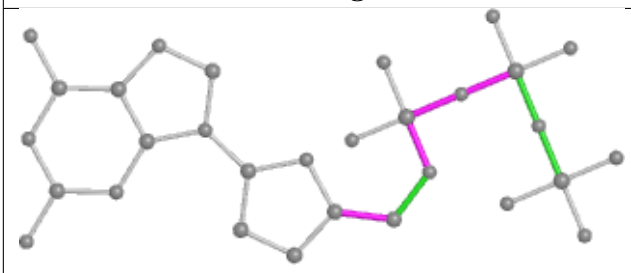
Ligand DG3 D 1583



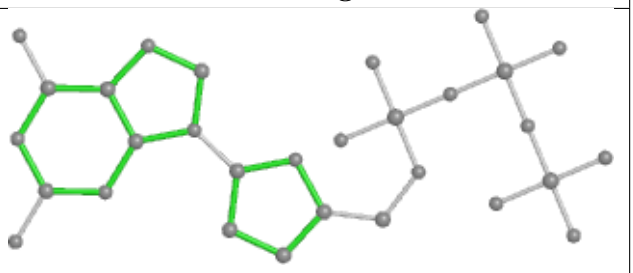
Bond lengths



Bond angles

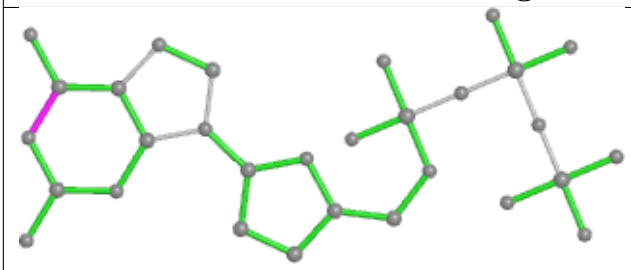


Torsions

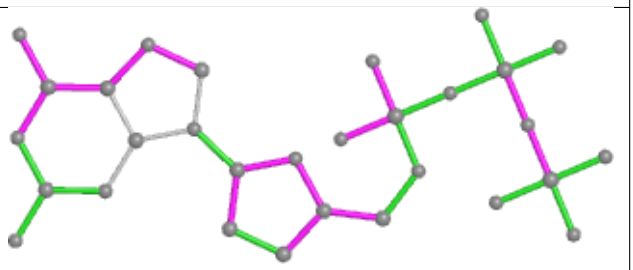


Rings

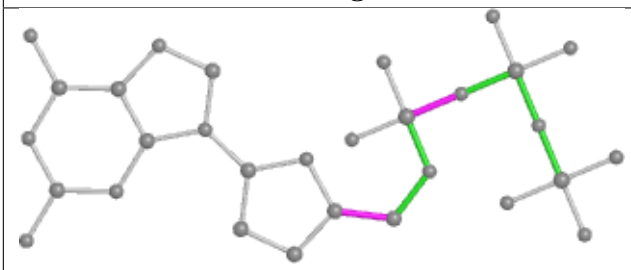
Ligand DG3 C 1585



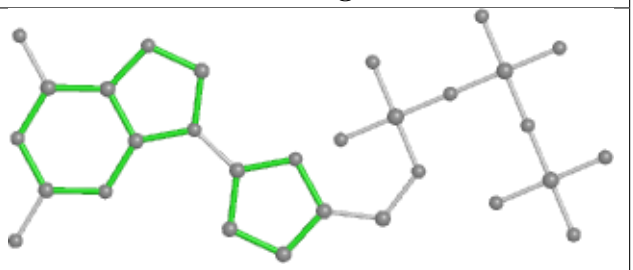
Bond lengths



Bond angles

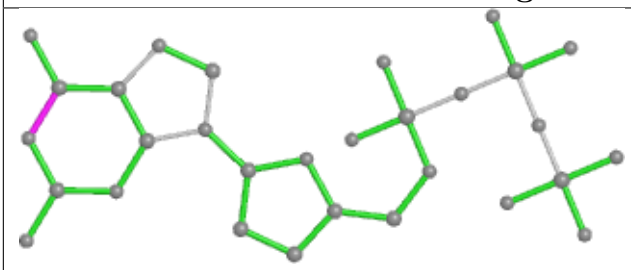


Torsions

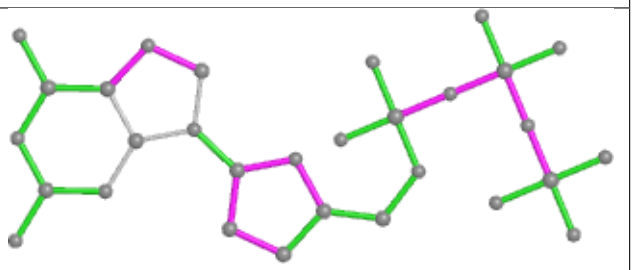


Rings

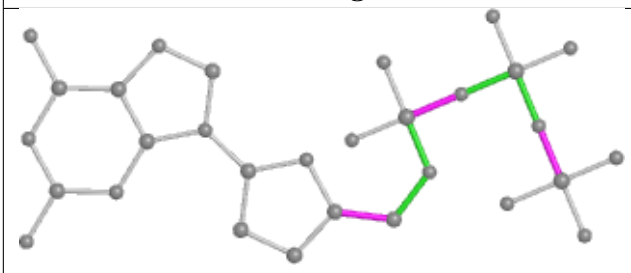
Ligand DG3 B 1584



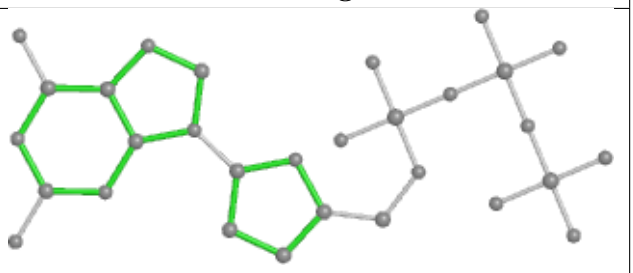
Bond lengths



Bond angles

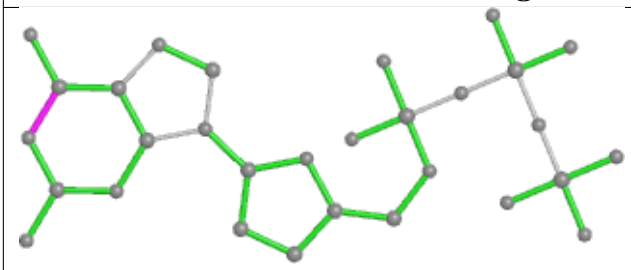


Torsions

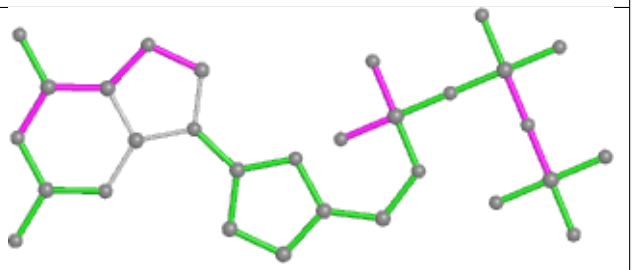


Rings

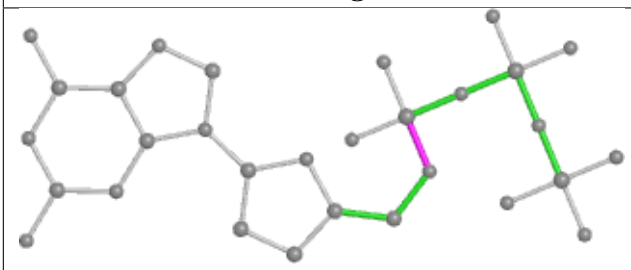
Ligand DG3 A 1585



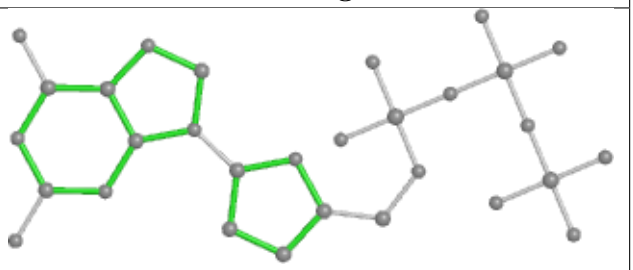
Bond lengths



Bond angles

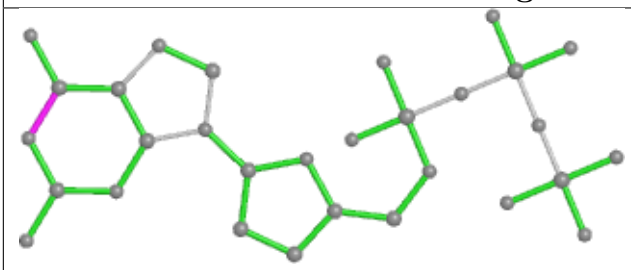


Torsions

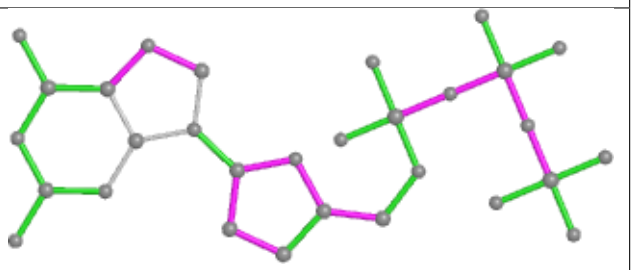


Rings

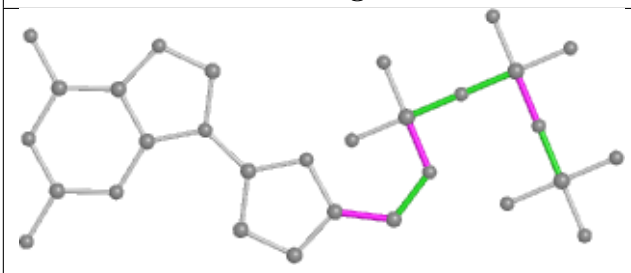
Ligand DG3 B 1588



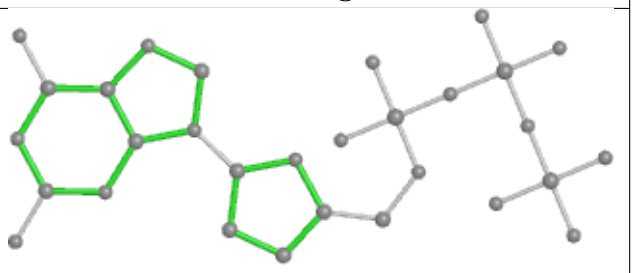
Bond lengths



Bond angles

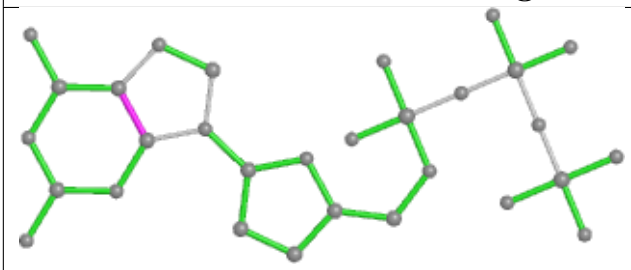


Torsions

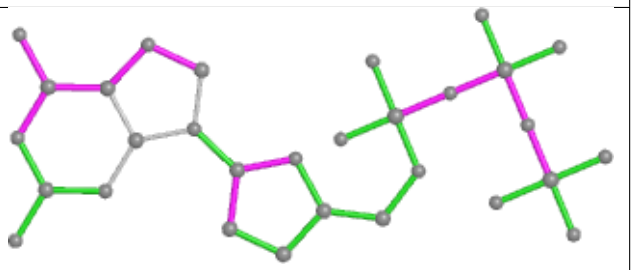


Rings

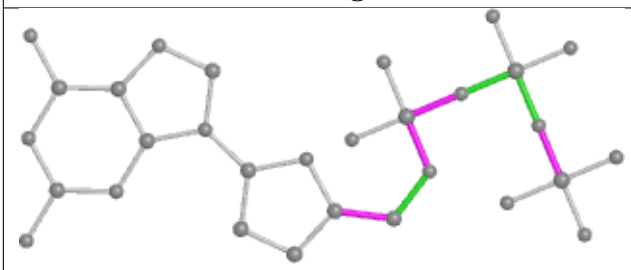
Ligand DG3 B 1587



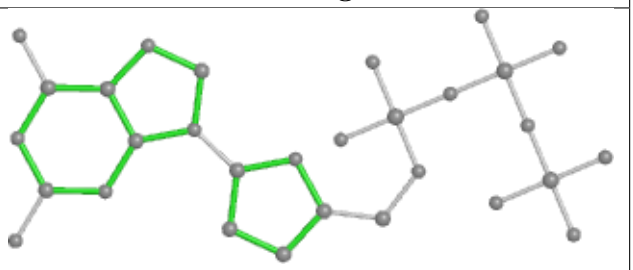
Bond lengths



Bond angles

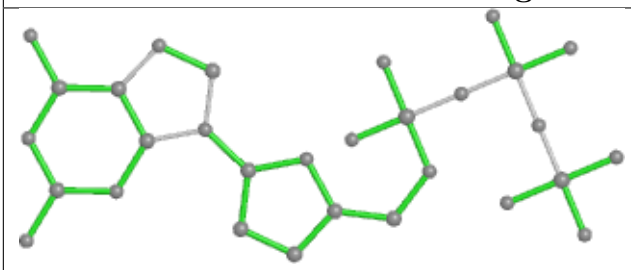


Torsions

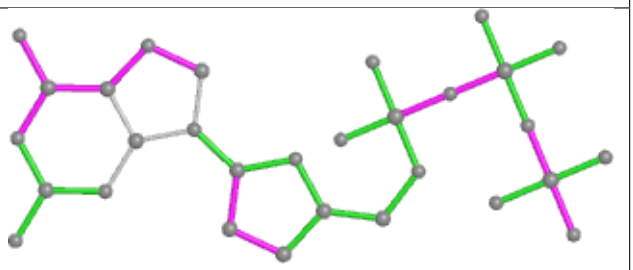


Rings

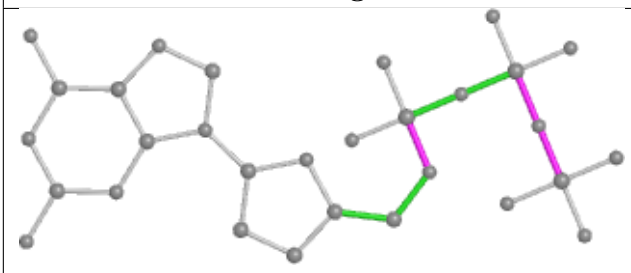
Ligand DG3 D 1586



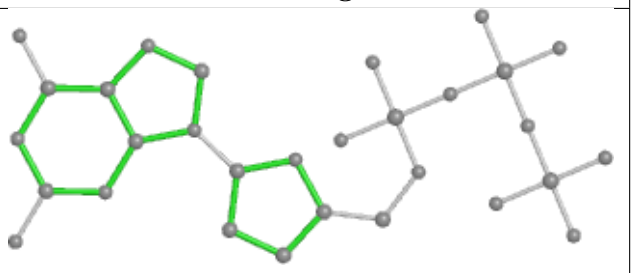
Bond lengths



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	457/491 (93%)	0.11	19 (4%)	36	42	31, 60, 108, 160	0
1	B	443/491 (90%)	0.07	16 (3%)	42	49	28, 58, 109, 152	0
1	C	457/491 (93%)	0.16	16 (3%)	44	51	34, 63, 107, 133	0
1	D	442/491 (90%)	0.03	13 (2%)	51	59	28, 57, 106, 142	0
All	All	1799/1964 (91%)	0.09	64 (3%)	42	49	28, 60, 108, 160	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	VAL	5.2
1	B	487	VAL	4.4
1	B	276	LEU	4.4
1	A	282	ASP	4.2
1	D	276	LEU	4.2
1	C	488	LEU	3.9
1	A	488	LEU	3.9
1	B	530	ILE	3.8
1	C	583	ASP	3.8
1	A	564	ALA	3.6
1	A	491	VAL	3.6
1	C	464	GLY	3.5
1	A	189	LEU	3.4
1	C	530	ILE	3.3
1	C	466	ILE	3.2
1	A	565	ALA	3.1
1	B	527	ASN	3.0
1	A	343	VAL	3.0
1	D	343	VAL	3.0
1	B	345	ASN	3.0
1	C	545	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	485	PRO	3.0
1	A	530	ILE	2.9
1	C	489	LEU	2.8
1	A	583	ASP	2.8
1	D	529	ALA	2.8
1	B	488	LEU	2.8
1	B	285	TRP	2.7
1	B	277	GLU	2.7
1	D	342	GLU	2.7
1	A	524	THR	2.6
1	B	291	PRO	2.6
1	B	583	ASP	2.6
1	D	530	ILE	2.6
1	B	557	VAL	2.5
1	C	341	CYS	2.5
1	A	490	ASP	2.5
1	B	341	CYS	2.5
1	D	341	CYS	2.5
1	B	259	LEU	2.5
1	C	490	ASP	2.5
1	A	552	VAL	2.4
1	D	466	ILE	2.4
1	D	515	ILE	2.4
1	C	487	VAL	2.4
1	D	521	TYR	2.4
1	C	266	CYS	2.4
1	A	562	LEU	2.3
1	D	345	ASN	2.3
1	C	284	LEU	2.3
1	B	506	ASP	2.3
1	C	343	VAL	2.3
1	C	515	ILE	2.2
1	B	284	LEU	2.2
1	C	514	PRO	2.2
1	D	114	GLY	2.2
1	A	493	LEU	2.2
1	D	284	LEU	2.2
1	A	259	LEU	2.1
1	A	360	TYR	2.0
1	B	513	ASN	2.0
1	C	540	LEU	2.0
1	A	284	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	113	PRO	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.

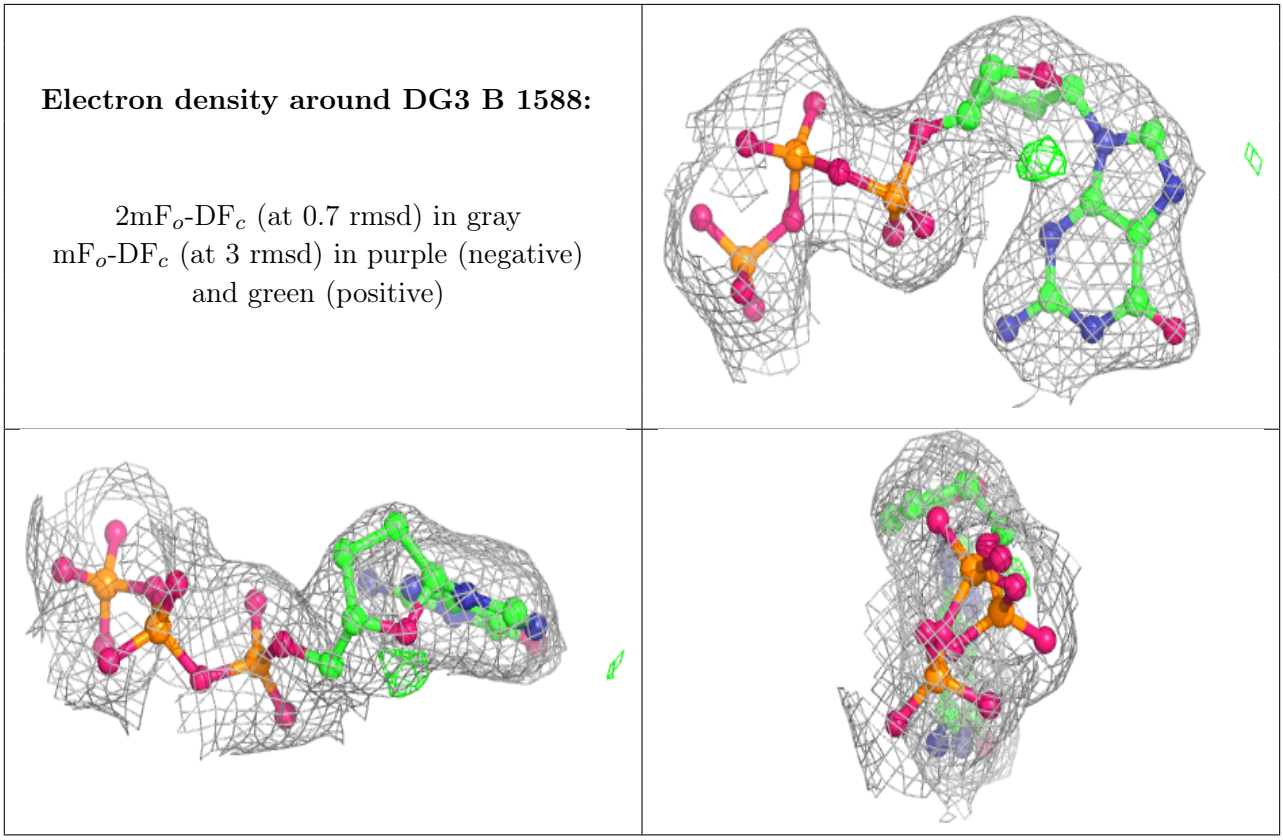
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1586	5/5	0.84	0.22	135,137,138,139	0
4	SO4	D	1588	5/5	0.85	0.20	135,137,138,140	0
4	SO4	D	1589	5/5	0.85	0.33	143,145,145,148	0
4	SO4	B	1589	5/5	0.88	0.14	139,141,141,142	0
5	MG	B	1585	1/1	0.88	0.13	84,84,84,84	0
5	MG	D	1584	1/1	0.91	0.15	85,85,85,85	0
5	MG	B	1590	1/1	0.94	0.15	74,74,74,74	0
3	DG3	B	1588	30/30	0.94	0.13	49,63,144,311	0
3	DG3	D	1587	30/30	0.95	0.12	53,65,161,351	0
3	DG3	B	1587	30/30	0.95	0.17	49,81,119,164	0
3	DG3	B	1584	30/30	0.95	0.12	39,58,108,215	0
3	DG3	D	1586	30/30	0.95	0.14	48,76,99,262	0
3	DG3	D	1583	30/30	0.96	0.16	47,57,150,179	0
3	DG3	A	1585	30/30	0.97	0.15	47,68,104,111	0
3	DG3	C	1585	30/30	0.97	0.13	48,66,120,265	0
5	MG	D	1590	1/1	0.98	0.06	84,84,84,84	0
2	FE	C	1584	1/1	0.99	0.11	51,51,51,51	0
2	FE	D	1585	1/1	0.99	0.09	39,39,39,39	0
2	FE	B	1586	1/1	0.99	0.12	42,42,42,42	0
2	FE	A	1584	1/1	1.00	0.13	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

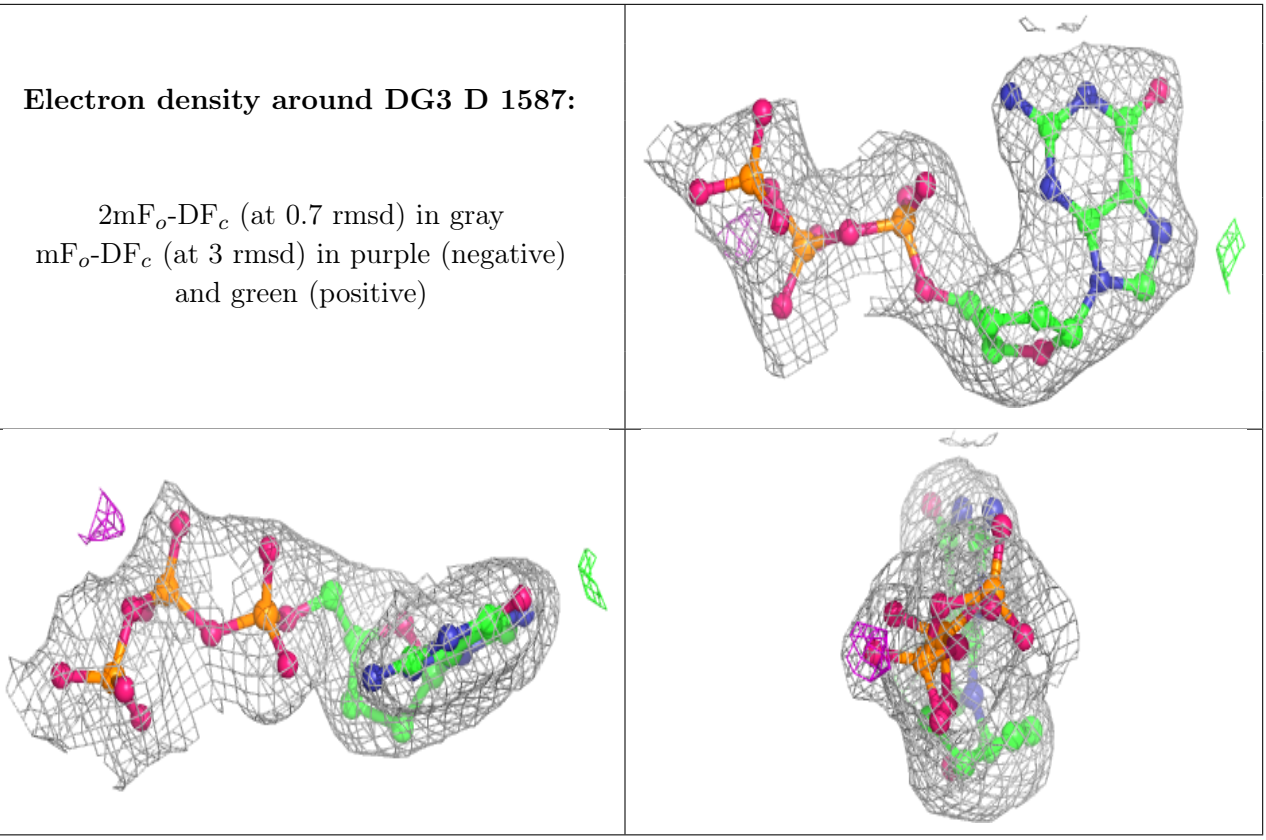
Electron density around DG3 B 1588:

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



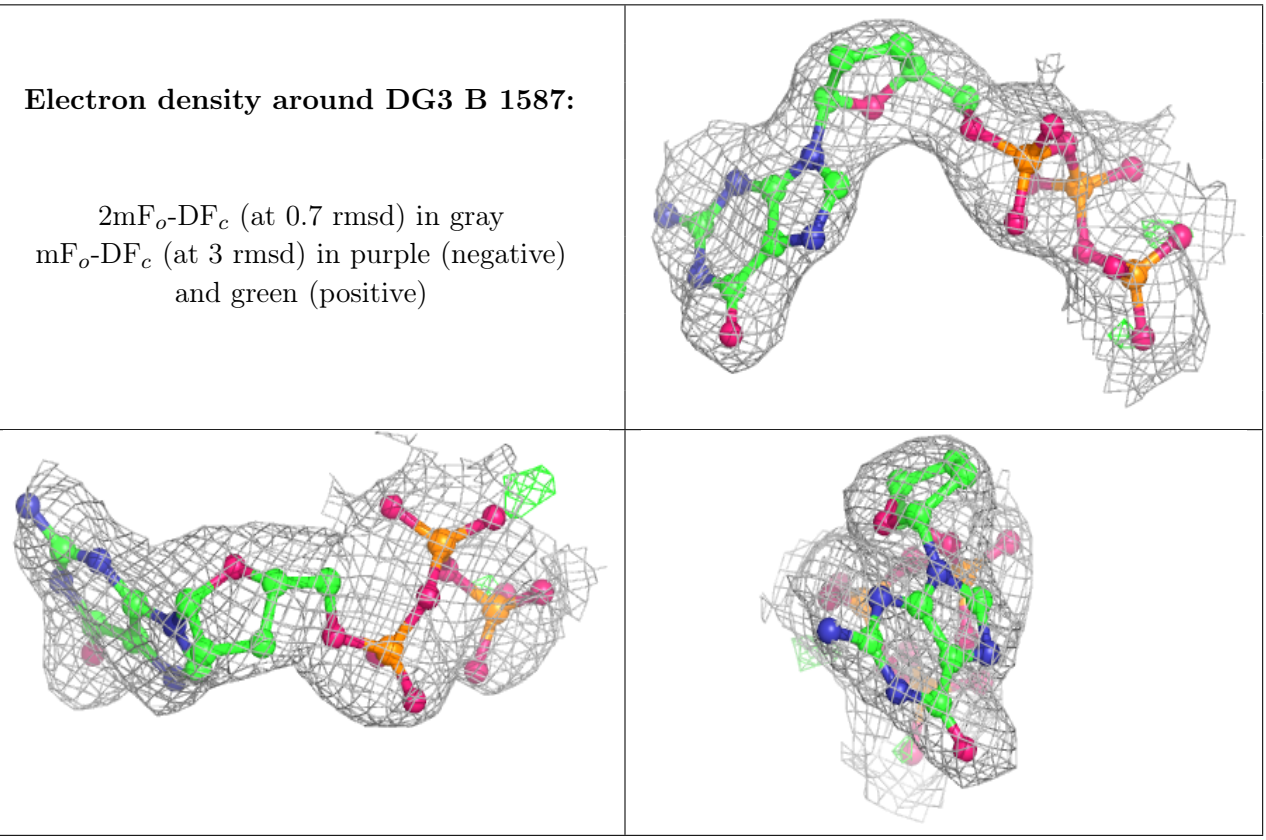
Electron density around DG3 D 1587:

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



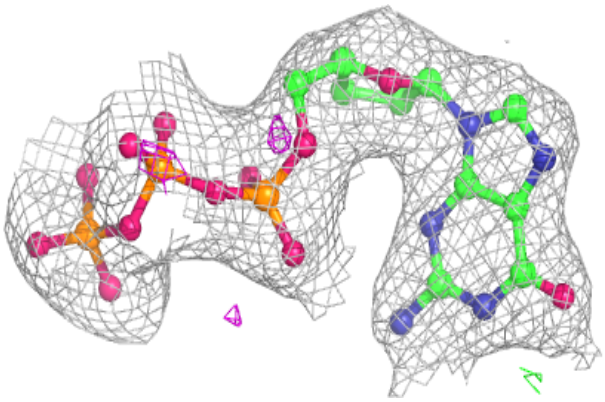
Electron density around DG3 B 1587:

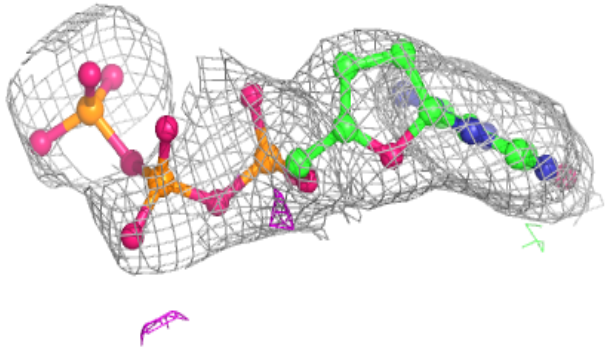
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

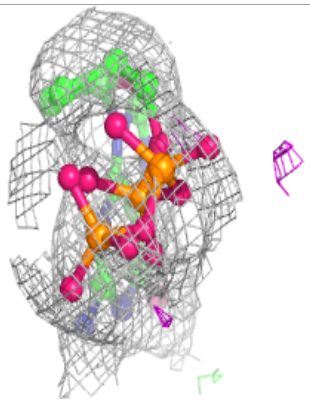


Electron density around DG3 B 1584:

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

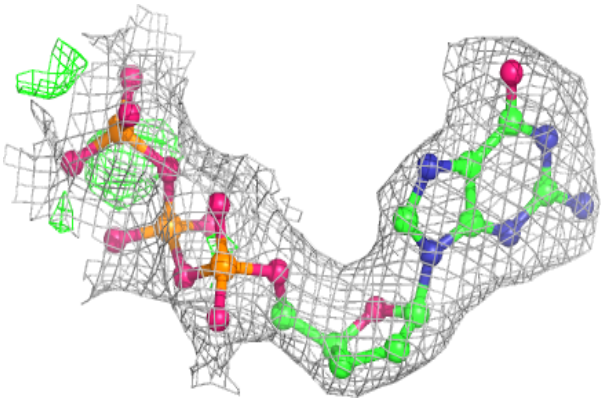


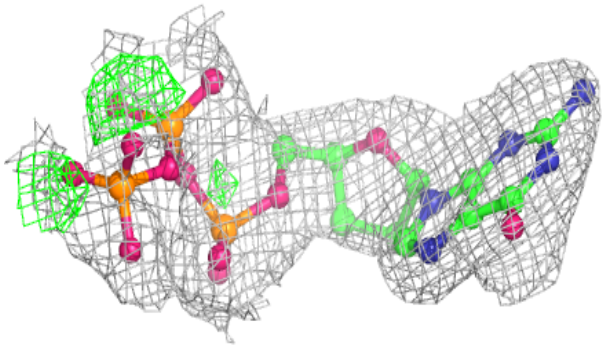


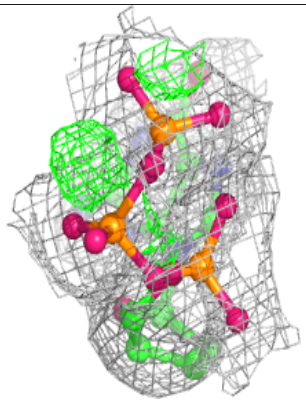


Electron density around DG3 D 1586:

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

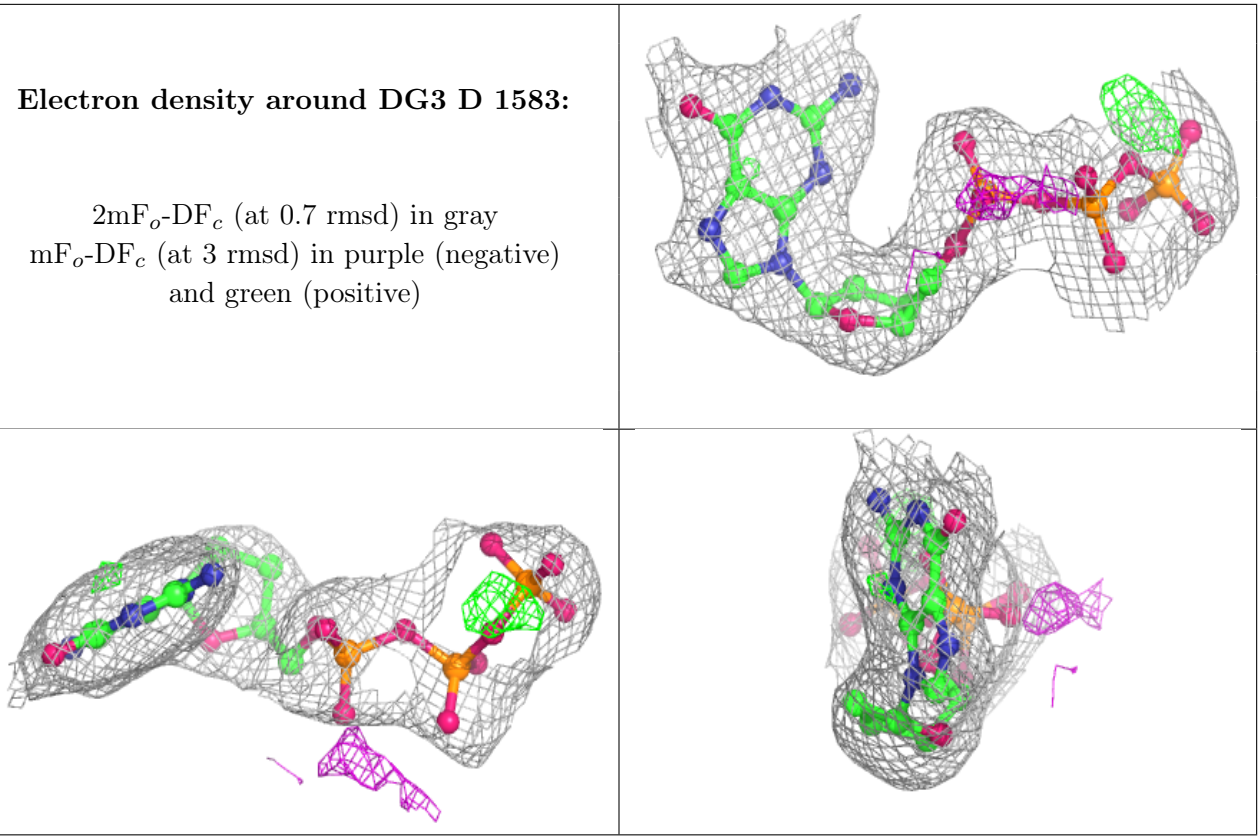






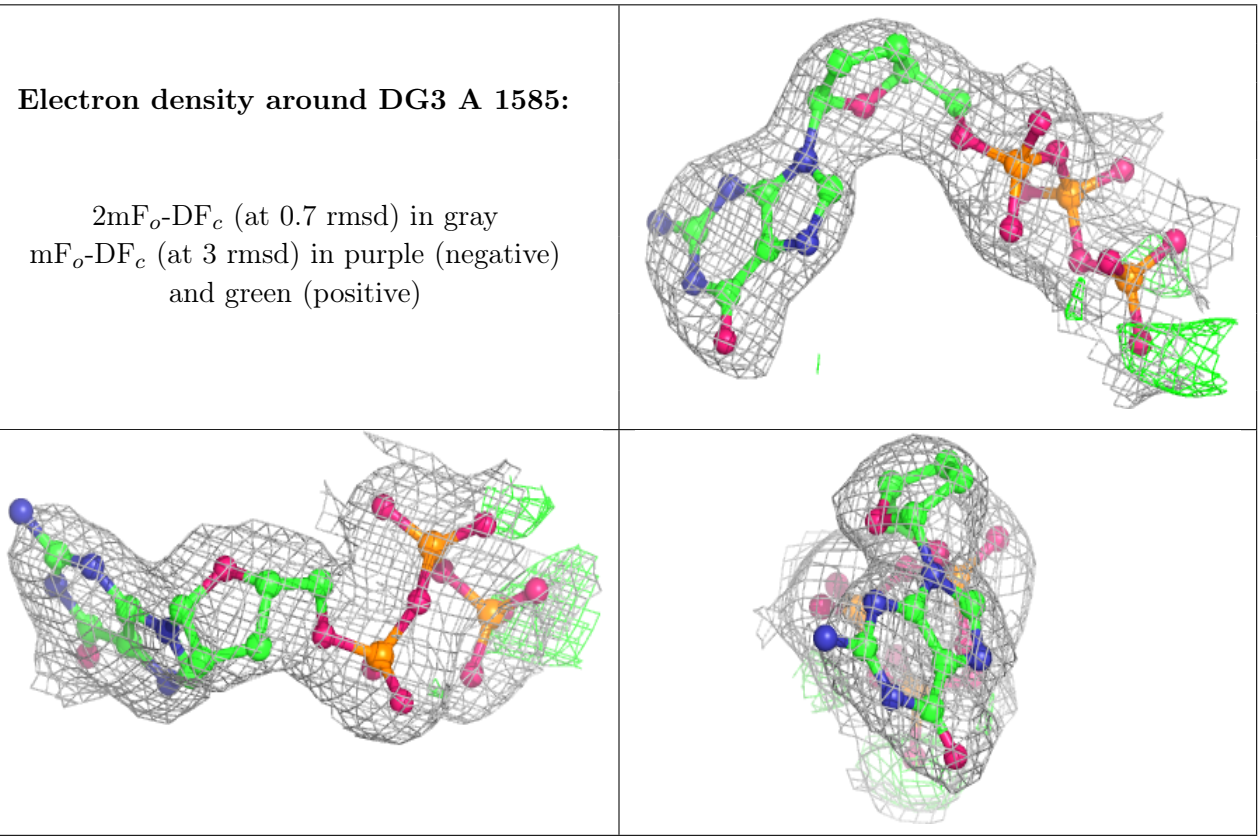
Electron density around DG3 D 1583:

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



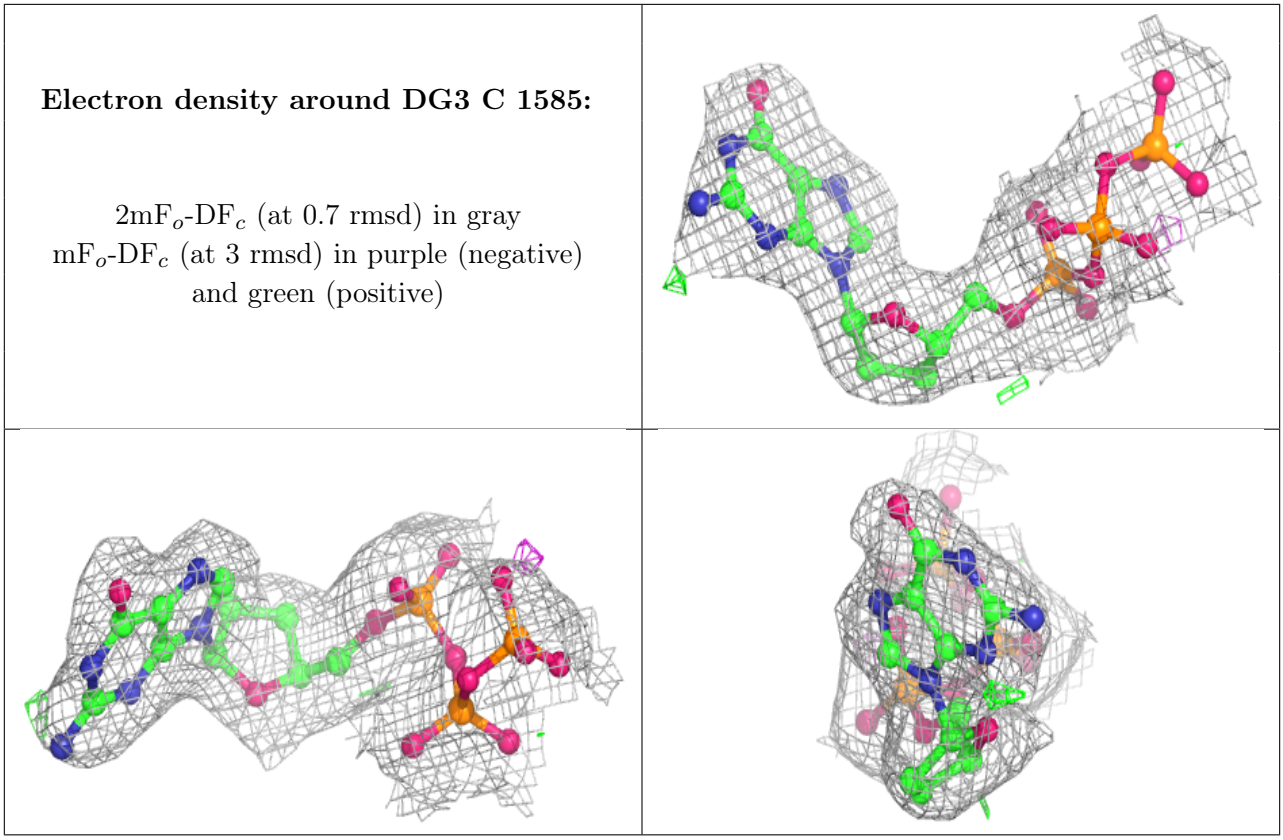
Electron density around DG3 A 1585:

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



Electron density around DG3 C 1585:

$2mF_o$-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.