



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:57 AM UTC

PDB ID : 5AO1 / pdb_00005ao1
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

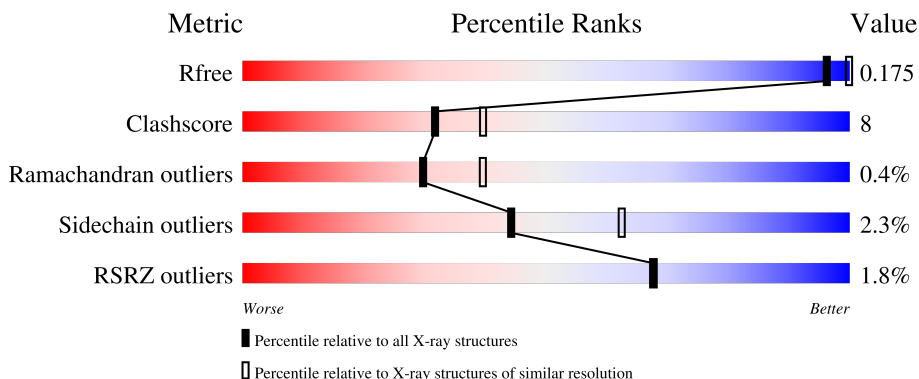
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	491	2% 75% 15% 7%
1	B	491	2% 69% 19% 10%
1	C	491	2% 74% 17% 7%
1	D	491	2% 76% 13% 10%

2 Entry composition

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 TRIPHOSPHO-HYDROLASE 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

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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

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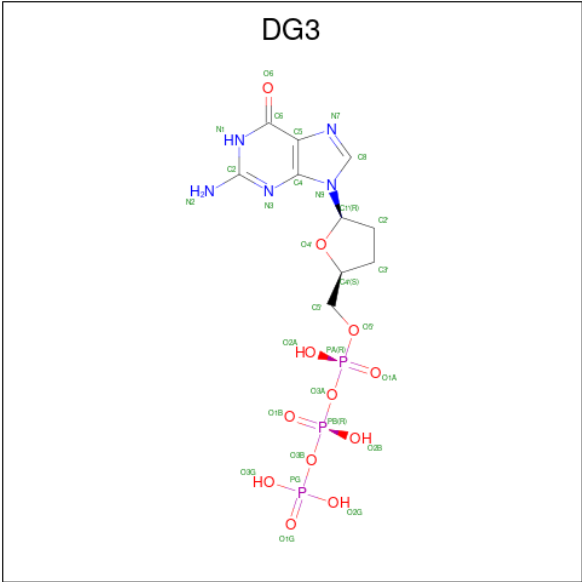
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Chain	Residue	Modelled	Actual	Comment	Reference
C	111	GLN	-	expression tag	UNP Q9Y3Z3
C	112	GLY	-	expression tag	UNP Q9Y3Z3
C	113	PRO	-	expression tag	UNP Q9Y3Z3
C	114	GLY	-	expression tag	UNP Q9Y3Z3
D	93	MET	-	expression tag	UNP Q9Y3Z3
D	94	ALA	-	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 (CCD ID: FE) (formula: Fe).

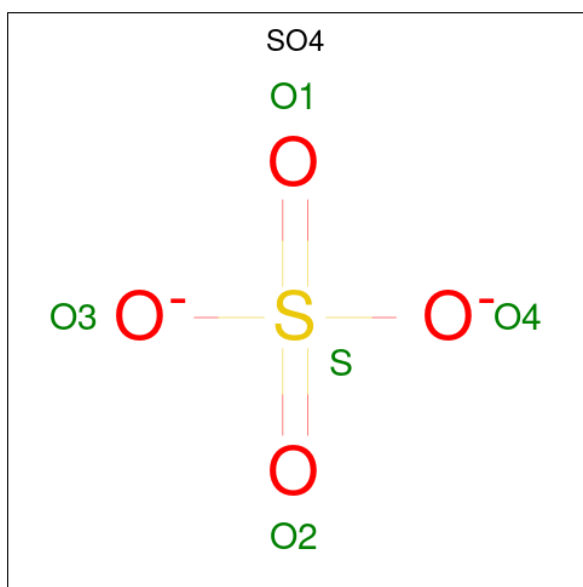
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DG3) (formula: C₁₀H₁₆N₅O₁₂P₃).



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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is water.

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

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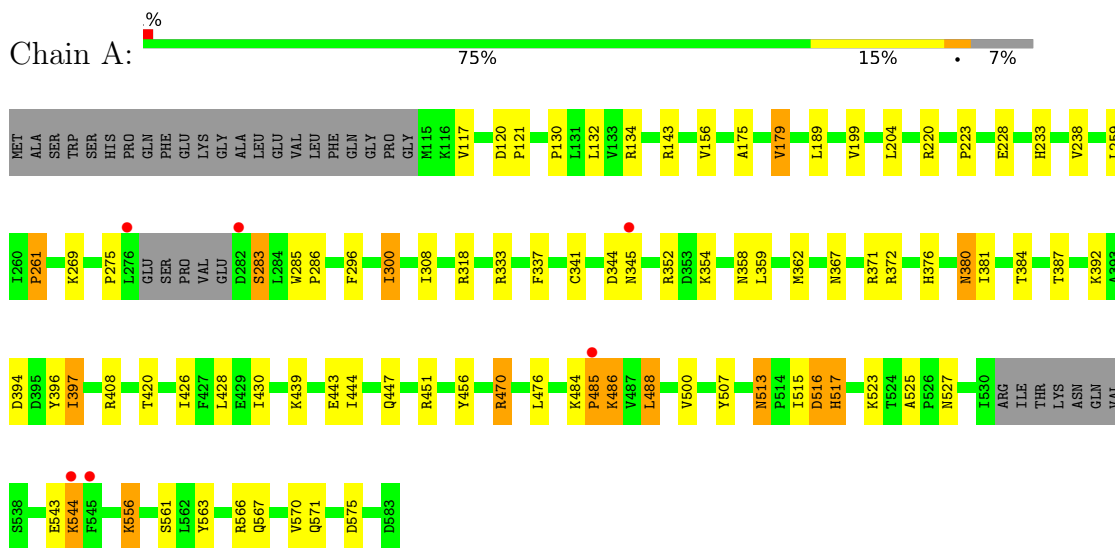
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	42	Total	O	0	0
			42	42		

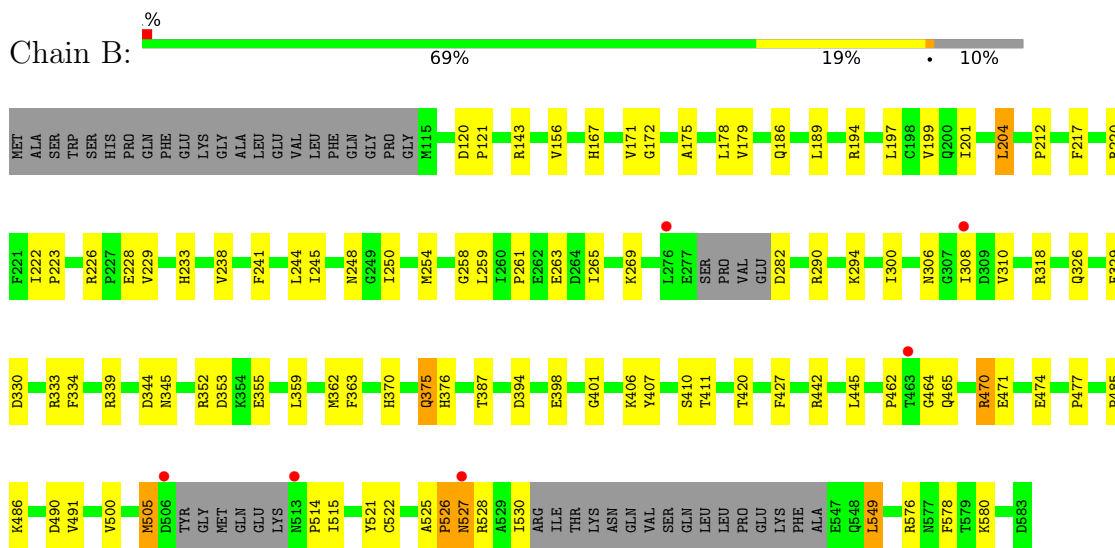
3 Residue-property plots

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

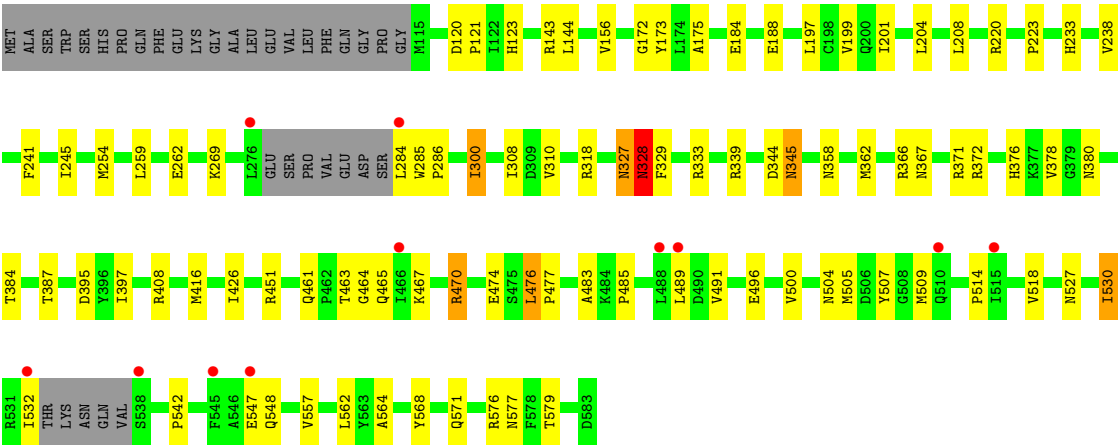


• Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

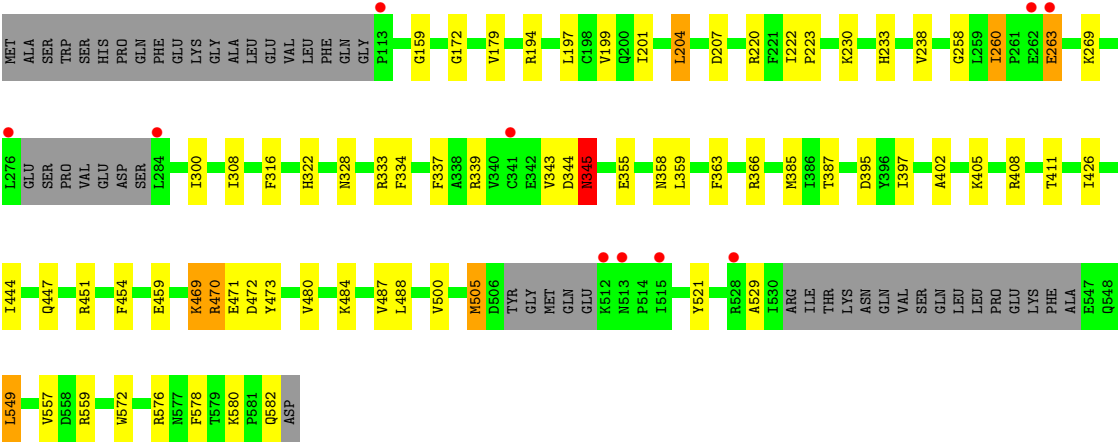
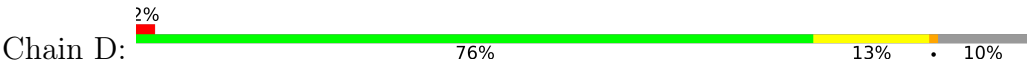


• Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1





● Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.171 , 0.220 0.177 , 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)	0.34 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	2/3692 (0.1%)	1.04	27/5002 (0.5%)
1	B	0.69	1/3558 (0.0%)	1.02	8/4827 (0.2%)
1	C	0.58	0/3701	0.98	11/5017 (0.2%)
1	D	0.67	3/3542 (0.1%)	1.08	12/4798 (0.3%)
All	All	0.65	6/14493 (0.0%)	1.03	58/19644 (0.3%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	263	GLU	CB-CG	8.87	1.79	1.52
1	B	222	ILE	CA-CB	7.48	1.58	1.54
1	D	222	ILE	CA-CB	6.85	1.58	1.53
1	D	260	ILE	CA-CB	-5.92	1.47	1.53
1	A	397	ILE	CA-CB	5.46	1.60	1.53
1	A	486	LYS	CA-C	5.27	1.59	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	484	LYS	CA-C-N	12.39	132.54	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	484	LYS	C-N-CA	12.39	132.54	119.78
1	D	263	GLU	N-CA-C	-10.62	98.56	112.68
1	D	580	LYS	CA-C-N	8.31	128.34	119.78
1	D	580	LYS	C-N-CA	8.31	128.34	119.78
1	C	344	ASP	CA-C-N	8.16	135.86	123.05
1	C	344	ASP	C-N-CA	8.16	135.86	123.05
1	C	327	ASN	CA-C-N	-8.04	109.79	122.65
1	C	327	ASN	C-N-CA	-8.04	109.79	122.65
1	A	525	ALA	CA-C-N	7.91	127.83	119.05
1	A	525	ALA	C-N-CA	7.91	127.83	119.05
1	A	543	GLU	CA-C-N	7.88	136.59	121.54
1	A	543	GLU	C-N-CA	7.88	136.59	121.54
1	A	345	ASN	N-CA-CB	-7.52	105.59	114.17
1	A	341	CYS	CA-C-N	6.82	131.06	121.24
1	A	341	CYS	C-N-CA	6.82	131.06	121.24
1	A	396	TYR	N-CA-C	6.78	121.71	113.17
1	D	469	LYS	CA-C-N	6.43	129.19	120.38
1	D	469	LYS	C-N-CA	6.43	129.19	120.38
1	D	345	ASN	N-CA-CB	-6.23	107.07	114.17
1	C	300	ILE	N-CA-C	6.13	116.32	110.74
1	D	300	ILE	N-CA-C	6.07	116.27	110.74
1	A	488	LEU	CA-CB-CG	6.03	137.39	116.30
1	C	483	ALA	N-CA-C	5.84	117.64	111.28
1	A	344	ASP	CA-C-N	-5.79	116.20	126.45
1	A	344	ASP	C-N-CA	-5.79	116.20	126.45
1	A	516	ASP	N-CA-C	-5.78	101.28	109.96
1	C	476	LEU	CA-C-N	-5.74	112.68	119.05
1	C	476	LEU	C-N-CA	-5.74	112.68	119.05
1	B	486	LYS	CA-C-N	-5.72	113.19	120.98
1	B	486	LYS	C-N-CA	-5.72	113.19	120.98
1	C	576	ARG	N-CA-C	-5.61	106.10	113.17
1	C	496	GLU	N-CA-C	-5.60	105.27	111.71
1	A	513	ASN	CA-C-N	5.59	125.20	119.56
1	A	513	ASN	C-N-CA	5.59	125.20	119.56
1	A	380	ASN	N-CA-C	5.56	117.42	111.36
1	D	260	ILE	CA-CB-CG2	-5.54	101.09	110.50
1	A	484	LYS	CA-C-N	5.53	126.75	119.84
1	A	484	LYS	C-N-CA	5.53	126.75	119.84
1	A	285	TRP	CA-C-N	5.50	125.20	119.64
1	A	285	TRP	C-N-CA	5.50	125.20	119.64
1	B	261	PRO	CA-C-N	-5.47	111.88	122.06
1	B	261	PRO	C-N-CA	-5.47	111.88	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	580	LYS	CA-C-N	5.41	125.33	119.76
1	B	580	LYS	C-N-CA	5.41	125.33	119.76
1	A	544	LYS	CA-C-N	-5.40	113.76	122.24
1	A	544	LYS	C-N-CA	-5.40	113.76	122.24
1	A	261	PRO	CA-C-N	-5.38	112.06	122.06
1	A	261	PRO	C-N-CA	-5.38	112.06	122.06
1	B	353	ASP	N-CA-C	5.33	117.09	111.28
1	A	300	ILE	N-CA-C	5.24	115.51	110.74
1	C	328	ASN	N-CA-C	-5.19	106.53	112.92
1	D	559	ARG	N-CA-C	5.17	117.58	111.33
1	A	485	PRO	CA-C-N	-5.14	113.27	122.07
1	A	485	PRO	C-N-CA	-5.14	113.27	122.07
1	A	488	LEU	CB-CG-CD1	5.06	125.88	110.70
1	D	488	LEU	N-CA-C	-5.05	102.57	110.10
1	B	485	PRO	N-CA-C	-5.01	103.33	111.14

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	47	0
1	B	3475	0	3271	63	0
1	C	3613	0	3427	64	0
1	D	3454	0	3266	54	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	D	42	0	0	6	0
All	All	14581	0	13485	227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (227) 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:CG	1:D:263:GLU:CB	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:N	1:C:328:ASN:HD22	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:B:254:MET:HE2	1:B:259:LEU:HD23	1.71	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:HG2	1:A:352:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:345:ASN:HD22	1.93	0.66
1:B:326:GLN:OE1	1:D:328:ASN:ND2	2.28	0.66
1:C:254:MET:HE2	1:C:259:LEU:HD23	1.78	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:469:LYS:HG3	1:D:471:GLU:CG	2.27	0.63
1:B:143:ARG:HD3	6:B:2002:HOH:O	1.98	0.62
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:D:263:GLU:CB	1:D:263:GLU:CD	2.72	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:B:228:GLU:H	1:B:228:GLU:CD	2.09	0.60
1:A:476:LEU:CB	1:A:500:VAL:HG11	2.31	0.60
1:D:230:LYS:NZ	6:D:2020:HOH:O	2.31	0.60
1:C:366:ARG:HG2	1:C:366:ARG:HH11	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:C:308:ILE:HG12	1:C:362:MET:HE1	1.83	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:B:308:ILE:HG12	1:B:362:MET:HE1	1.87	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:330:ASP:CG	1:B:333:ARG:HG3	2.31	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:C:328:ASN:N	1:C:328:ASN:ND2	2.47	0.55
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:B:505:MET:HE2	1:B:549:LEU:HD23	1.91	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
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: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:C:416:MET:HE2	1:C:416:MET:HA	1.94	0.49
1:A:392:LYS:NZ	1:A:444:ILE:HD11	2.27	0.49
1:B:156:VAL:HG11	1:B:376:HIS:CE1	2.48	0.49
1:B:156:VAL:O	3:B:1584:DG3:H8	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:408:ARG:H	1:D:411:THR:HG1	1.60	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:C:467:LYS:HB3	1:C:548:GLN:CD	2.38	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:308:ILE:HG12	1:A:362:MET:HE1	1.95	0.47
1:A:397:ILE:HD11	1:A:430:ILE:HG12	1.96	0.47
1:C:509:MET:HE3	1:C:509:MET:HB3	1.63	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
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:188:GLU:H	1:C:188:GLU:CD	2.24	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:C:327:ASN:C	1:C:328:ASN:HD22	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:505[A]:MET:HE2	6:D:2038:HOH:O	2.16	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:525:ALA:C	1:B:526:PRO:O	2.59	0.44
1:C:367:ASN:CG	1:C:542:PRO:HB3	2.42	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:C:505:MET:HE3	1:C:547:GLU:CD	2.43	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:514:PRO:O	1:C:518:VAL:HG23	2.18	0.43
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:OD1	1:D:345:ASN:O	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:HD23	1:B:359:LEU:HA	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:C:463:THR:C	1:C:465:GLN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:489:LEU:HD13	1:C:491:VAL:C	2.46	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:516:ASP:C	1:A:517:HIS:HD1	2.27	0.41
1:B:526:PRO:C	1:B:528:ARG:H	2.28	0.41
1:A:143:ARG:HD2	1:A:420:THR:HA	2.03	0.40
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:B:306:ASN:OD1	1:B:306:ASN:C	2.64	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:A:556:LYS:HZ3	1:A:561:SER:CB	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	18	25
1	B	435/491 (89%)	422 (97%)	10 (2%)	3 (1%)	18	25
1	C	451/491 (92%)	443 (98%)	7 (2%)	1 (0%)	43	56
1	D	435/491 (89%)	428 (98%)	7 (2%)	0	100	100
All	All	1773/1964 (90%)	1734 (98%)	32 (2%)	7 (0%)	30	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	B	465	GLN
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%)	362 (98%)	8 (2%)	45	64
1	B	356/434 (82%)	343 (96%)	13 (4%)	30	45
1	C	372/434 (86%)	366 (98%)	6 (2%)	55	73
1	D	351/434 (81%)	343 (98%)	8 (2%)	44	62
All	All	1449/1736 (84%)	1414 (98%)	35 (2%)	44	61

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
1	A	179	VAL
1	A	228	GLU
1	A	283	SER
1	A	354	LYS
1	A	470	ARG
1	A	488	LEU
1	A	556	LYS
1	B	179	VAL
1	B	204	LEU
1	B	229	VAL
1	B	282	ASP
1	B	375	GLN
1	B	470	ARG
1	B	471	GLU
1	B	490	ASP
1	B	491	VAL
1	B	505	MET
1	B	515	ILE
1	B	527	ASN
1	B	549	LEU
1	C	184	GLU
1	C	262	GLU
1	C	328	ASN
1	C	345	ASN
1	C	470	ARG
1	C	530	ILE
1	D	204	LEU
1	D	345	ASN
1	D	470	ARG

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Mol	Chain	Res	Type
1	D	487	VAL
1	D	505[A]	MET
1	D	505[B]	MET
1	D	549	LEU
1	D	582	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	425	ASN
1	B	149	GLN
1	B	200	GLN
1	B	235	GLN
1	B	364	HIS
1	B	380	ASN
1	B	452	ASN
1	C	200	GLN
1	C	345	ASN
1	C	367	ASN
1	C	465	GLN
1	D	200	GLN
1	D	321	HIS
1	D	364	HIS
1	D	571	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	1587	2	31,32,32	1.31	2 (6%)	44,50,50	1.83	8 (18%)
4	SO4	A	1586	-	4,4,4	0.27	0	6,6,6	0.14	0
3	DG3	B	1584	5	31,32,32	1.42	4 (12%)	44,50,50	1.92	10 (22%)
3	DG3	D	1586	2	31,32,32	1.29	3 (9%)	44,50,50	1.90	8 (18%)
3	DG3	D	1587	5	31,32,32	1.42	6 (19%)	44,50,50	1.83	6 (13%)
3	DG3	B	1588	5	31,32,32	1.59	6 (19%)	44,50,50	2.07	12 (27%)
3	DG3	A	1585	2	31,32,32	1.40	5 (16%)	44,50,50	2.00	9 (20%)
4	SO4	B	1589	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	D	1588	-	4,4,4	0.26	0	6,6,6	0.20	0
3	DG3	C	1585	2	31,32,32	1.29	4 (12%)	44,50,50	1.99	13 (29%)
4	SO4	D	1589	-	4,4,4	0.26	0	6,6,6	0.46	0
3	DG3	D	1583	5	31,32,32	1.28	4 (12%)	44,50,50	2.03	11 (25%)

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	B	1587	2	-	6/22/31/31	0/3/3/3
3	DG3	B	1584	5	-	8/22/31/31	0/3/3/3
3	DG3	D	1586	2	-	5/22/31/31	0/3/3/3
3	DG3	D	1587	5	-	6/22/31/31	0/3/3/3
3	DG3	B	1588	5	-	7/22/31/31	0/3/3/3
3	DG3	A	1585	2	-	3/22/31/31	0/3/3/3
3	DG3	C	1585	2	-	2/22/31/31	0/3/3/3
3	DG3	D	1583	5	-	9/22/31/31	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1588	DG3	PB-O3A	4.02	1.63	1.59
3	A	1585	DG3	PB-O3B	3.86	1.63	1.59
3	B	1588	DG3	PA-O3A	3.84	1.63	1.59
3	B	1587	DG3	C5-C4	3.49	1.48	1.38
3	B	1584	DG3	PA-O3A	3.38	1.63	1.59
3	D	1587	DG3	C5-C4	3.33	1.47	1.38
3	B	1587	DG3	PB-O3B	3.21	1.63	1.59
3	B	1584	DG3	PB-O3A	3.21	1.63	1.59
3	D	1586	DG3	C5-C4	3.17	1.47	1.38
3	B	1584	DG3	C5-C4	3.11	1.47	1.38
3	C	1585	DG3	PB-O3B	3.07	1.62	1.59
3	D	1587	DG3	PB-O3A	3.00	1.62	1.59
3	A	1585	DG3	C5-C4	3.00	1.47	1.38
3	D	1583	DG3	C5-C4	2.97	1.46	1.38
3	B	1588	DG3	C5-C4	2.96	1.46	1.38
3	B	1584	DG3	C6-N1	-2.95	1.33	1.38
3	C	1585	DG3	C5-C4	2.90	1.46	1.38
3	B	1588	DG3	PB-O3B	2.88	1.62	1.59
3	D	1586	DG3	PA-O3A	2.88	1.62	1.59
3	D	1587	DG3	PB-O3B	2.80	1.62	1.59
3	D	1587	DG3	PA-O3A	2.70	1.62	1.59
3	D	1587	DG3	C6-N1	-2.60	1.34	1.38
3	A	1585	DG3	C6-N1	-2.57	1.34	1.38
3	D	1583	DG3	C6-N1	-2.42	1.34	1.38
3	A	1585	DG3	PB-O3A	2.40	1.62	1.59
3	D	1583	DG3	C5-N7	-2.29	1.34	1.39
3	A	1585	DG3	C5-N7	-2.28	1.34	1.39
3	B	1588	DG3	C5-N7	-2.24	1.34	1.39
3	D	1586	DG3	PB-O3A	2.24	1.61	1.59
3	C	1585	DG3	C6-N1	-2.19	1.34	1.38
3	D	1583	DG3	PB-O3B	2.19	1.61	1.59
3	B	1588	DG3	C6-N1	-2.15	1.34	1.38
3	D	1587	DG3	C5-N7	-2.11	1.34	1.39
3	C	1585	DG3	C5-N7	-2.10	1.34	1.39

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1583	DG3	C5-C4-N3	-6.42	118.17	128.39
3	B	1588	DG3	C5-C4-N3	-6.33	118.31	128.39
3	D	1587	DG3	C5-C4-N3	-6.32	118.34	128.39
3	A	1585	DG3	C5-C4-N3	-6.23	118.48	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1584	DG3	C5-C4-N3	-6.04	118.78	128.39
3	D	1586	DG3	C5-C4-N3	-5.73	119.26	128.39
3	C	1585	DG3	C5-C4-N3	-5.68	119.35	128.39
3	B	1587	DG3	C5-C4-N3	-5.41	119.77	128.39
3	B	1584	DG3	C2-N3-C4	5.36	121.53	112.30
3	B	1588	DG3	C2-N3-C4	5.09	121.06	112.30
3	D	1583	DG3	N9-C4-N3	5.03	136.01	125.95
3	B	1588	DG3	N9-C4-N3	5.01	135.97	125.95
3	C	1585	DG3	C2-N3-C4	5.00	120.92	112.30
3	A	1585	DG3	C2-N3-C4	5.00	120.90	112.30
3	D	1583	DG3	C2-N3-C4	4.93	120.80	112.30
3	D	1587	DG3	C2-N3-C4	4.88	120.71	112.30
3	D	1586	DG3	C2-N3-C4	4.85	120.66	112.30
3	D	1587	DG3	N9-C4-N3	4.68	135.32	125.95
3	B	1587	DG3	C2-N3-C4	4.60	120.23	112.30
3	A	1585	DG3	N9-C4-N3	4.46	134.87	125.95
3	D	1586	DG3	N9-C4-N3	4.41	134.78	125.95
3	B	1584	DG3	N9-C4-N3	4.38	134.71	125.95
3	C	1585	DG3	N9-C4-N3	4.20	134.36	125.95
3	B	1587	DG3	N9-C4-N3	4.12	134.20	125.95
3	B	1584	DG3	C6-C5-N7	3.62	136.87	130.29
3	C	1585	DG3	C6-C5-N7	3.39	136.47	130.29
3	B	1588	DG3	O4'-C4'-C5'	-3.38	103.24	109.34
3	A	1585	DG3	C6-C5-N7	3.26	136.22	130.29
3	B	1587	DG3	C6-C5-N7	3.17	136.06	130.29
3	D	1586	DG3	C6-C5-N7	3.05	135.85	130.29
3	D	1587	DG3	C6-C5-N7	2.88	135.54	130.29
3	B	1588	DG3	C6-C5-N7	2.88	135.54	130.29
3	B	1584	DG3	C4-C5-N7	-2.88	106.11	110.67
3	A	1585	DG3	C4-C5-N7	-2.87	106.11	110.67
3	A	1585	DG3	O3A-PA-O1A	-2.79	102.33	110.70
3	D	1583	DG3	C4-C5-N7	-2.77	106.28	110.67
3	A	1585	DG3	O3A-PB-O1B	-2.77	102.38	110.70
3	B	1588	DG3	C4-C5-N7	-2.75	106.31	110.67
3	C	1585	DG3	O4'-C4'-C5'	-2.74	104.40	109.34
3	D	1583	DG3	C6-C5-N7	2.72	135.25	130.29
3	D	1583	DG3	C3'-C2'-C1'	2.69	105.97	102.87
3	D	1586	DG3	O6-C6-C5	-2.67	119.49	126.53
3	D	1587	DG3	C4-C5-N7	-2.64	106.49	110.67
3	C	1585	DG3	O6-C6-C5	-2.64	119.57	126.53
3	C	1585	DG3	C4-C5-N7	-2.61	106.53	110.67
3	B	1588	DG3	C4'-O4'-C1'	2.59	112.25	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1587	DG3	C4-C5-N7	-2.54	106.65	110.67
3	B	1588	DG3	O2A-PA-O3A	2.53	114.12	107.27
3	B	1587	DG3	O6-C6-C5	-2.53	119.86	126.53
3	B	1584	DG3	C4'-O4'-C1'	-2.51	107.44	109.81
3	D	1586	DG3	C4-C5-N7	-2.44	106.80	110.67
3	D	1583	DG3	O4'-C4'-C3'	2.43	108.81	104.81
3	D	1583	DG3	C8-N7-C5	2.42	108.57	104.26
3	B	1584	DG3	C3'-C2'-C1'	2.38	105.61	102.87
3	D	1583	DG3	C1'-N9-C8	-2.36	122.61	127.91
3	C	1585	DG3	O4'-C1'-C2'	2.34	109.19	106.41
3	D	1587	DG3	C3'-C2'-C1'	2.30	105.52	102.87
3	B	1588	DG3	C3'-C2'-C1'	2.22	105.43	102.87
3	B	1588	DG3	O6-C6-C5	-2.22	120.68	126.53
3	C	1585	DG3	O3A-PA-O1A	-2.22	104.03	110.70
3	B	1587	DG3	O3A-PA-O1A	-2.21	104.04	110.70
3	B	1588	DG3	C1'-N9-C8	-2.19	123.01	127.91
3	A	1585	DG3	O2A-PA-O1A	2.18	122.57	112.44
3	A	1585	DG3	C8-N7-C5	2.17	108.13	104.26
3	D	1586	DG3	O2A-PA-O3A	2.14	113.05	107.27
3	D	1583	DG3	O2A-PA-O3A	2.13	113.04	107.27
3	B	1588	DG3	C8-N7-C5	2.11	108.01	104.26
3	C	1585	DG3	O2A-PA-O3A	2.10	112.95	107.27
3	D	1583	DG3	O6-C6-C5	-2.10	120.99	126.53
3	C	1585	DG3	O3A-PB-O1B	-2.10	104.39	110.70
3	C	1585	DG3	O2A-PA-O1A	2.10	122.19	112.44
3	C	1585	DG3	O4'-C4'-C3'	2.08	108.23	104.81
3	D	1586	DG3	O2G-PG-O3B	-2.06	97.72	104.64
3	B	1587	DG3	O4'-C1'-C2'	2.06	108.85	106.41
3	B	1584	DG3	O3B-PG-O1G	-2.04	100.28	111.04
3	B	1584	DG3	O2A-PA-O1A	2.02	121.84	112.44
3	B	1584	DG3	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

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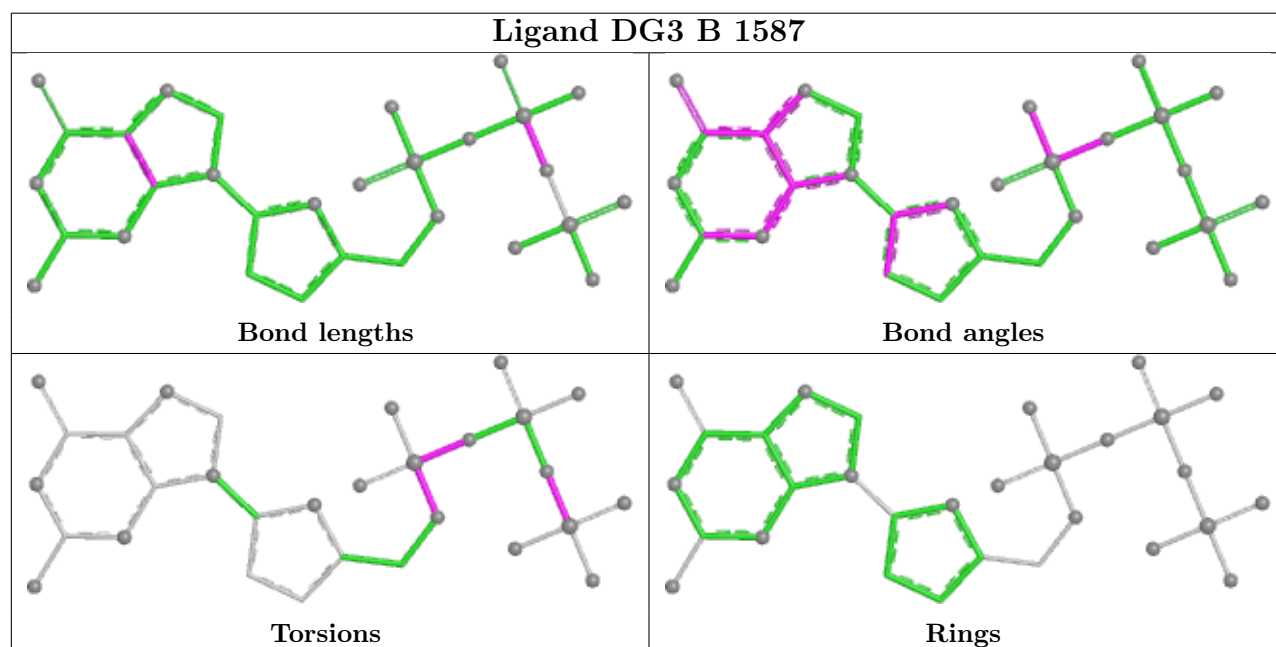
Mol	Chain	Res	Type	Atoms
3	D	1583	DG3	C5'-O5'-PA-O3A
3	D	1583	DG3	C5'-O5'-PA-O1A
3	D	1583	DG3	C5'-O5'-PA-O2A
3	D	1583	DG3	O4'-C4'-C5'-O5'
3	D	1583	DG3	C3'-C4'-C5'-O5'
3	D	1586	DG3	C5'-O5'-PA-O1A
3	D	1587	DG3	PB-O3B-PG-O2G
3	B	1584	DG3	O4'-C4'-C5'-O5'
3	D	1583	DG3	C2'-C1'-N9-C4
3	D	1583	DG3	C2'-C1'-N9-C8
3	D	1586	DG3	PG-O3B-PB-O1B
3	B	1588	DG3	C2'-C1'-N9-C4
3	D	1587	DG3	C2'-C1'-N9-C4
3	A	1585	DG3	C5'-O5'-PA-O3A
3	A	1585	DG3	C5'-O5'-PA-O1A
3	A	1585	DG3	C5'-O5'-PA-O2A
3	B	1584	DG3	C2'-C1'-N9-C8
3	B	1588	DG3	C5'-O5'-PA-O1A
3	D	1586	DG3	C5'-O5'-PA-O3A
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	1584	DG3	C2'-C1'-N9-C4
3	B	1588	DG3	C2'-C1'-N9-C8
3	D	1587	DG3	C2'-C1'-N9-C8
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	D	1586	DG3	PB-O3B-PG-O3G
3	D	1587	DG3	PB-O3B-PG-O3G
3	B	1584	DG3	C3'-C4'-C5'-O5'
3	C	1585	DG3	O4'-C4'-C5'-O5'
3	C	1585	DG3	PB-O3A-PA-O2A
3	D	1583	DG3	PA-O3A-PB-O1B
3	D	1586	DG3	PG-O3B-PB-O2B
3	B	1584	DG3	PB-O3A-PA-O2A
3	B	1588	DG3	PG-O3B-PB-O2B
3	D	1587	DG3	PA-O3A-PB-O2B

There are no ring outliers.

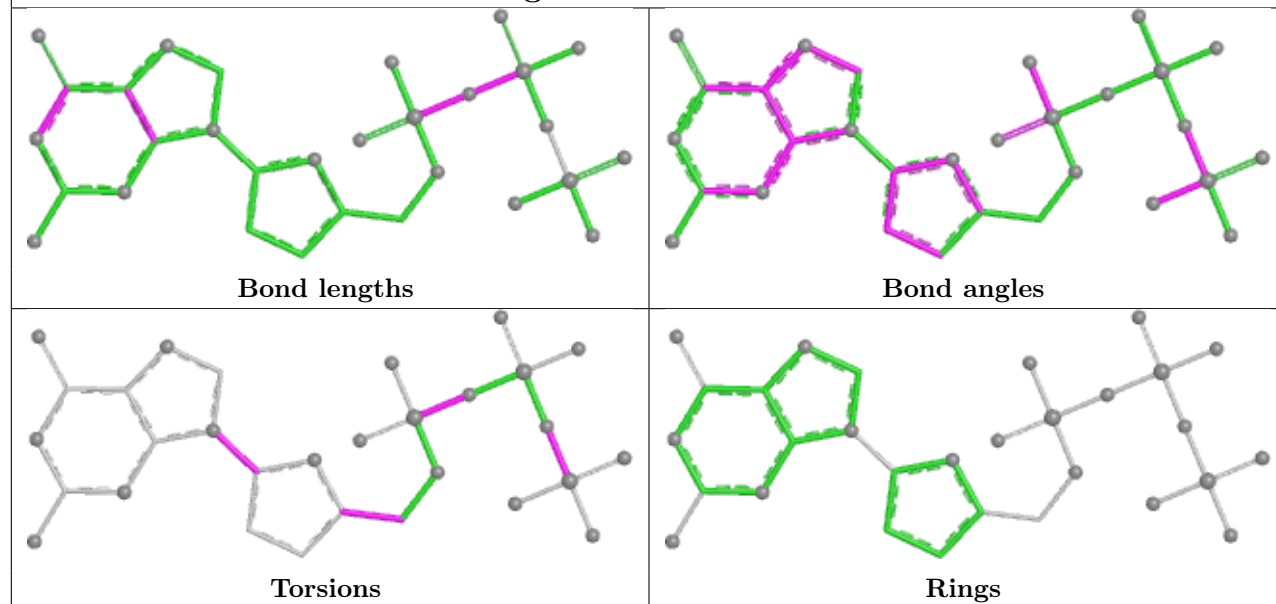
10 monomers are involved in 16 short contacts:

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

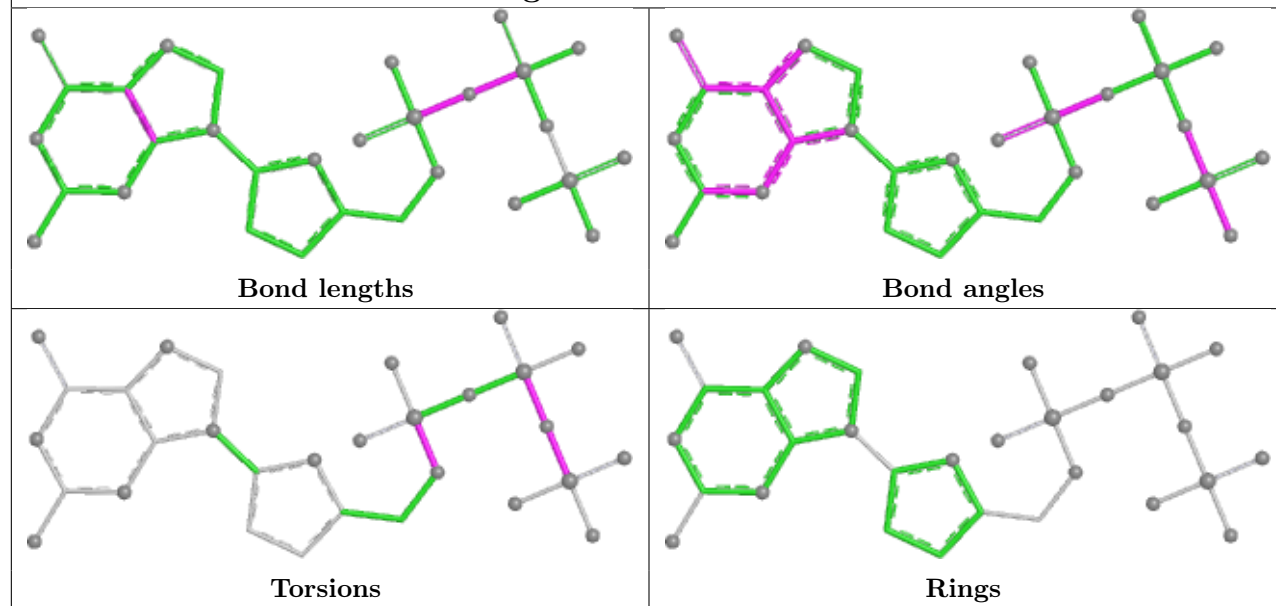
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

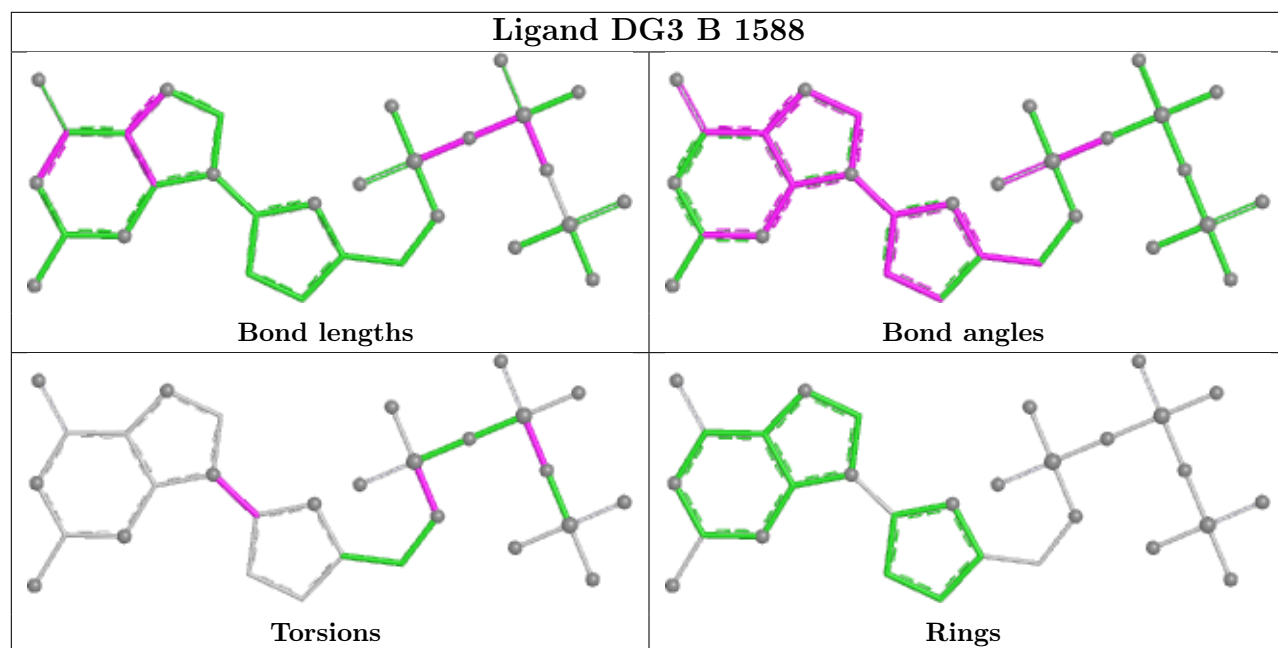
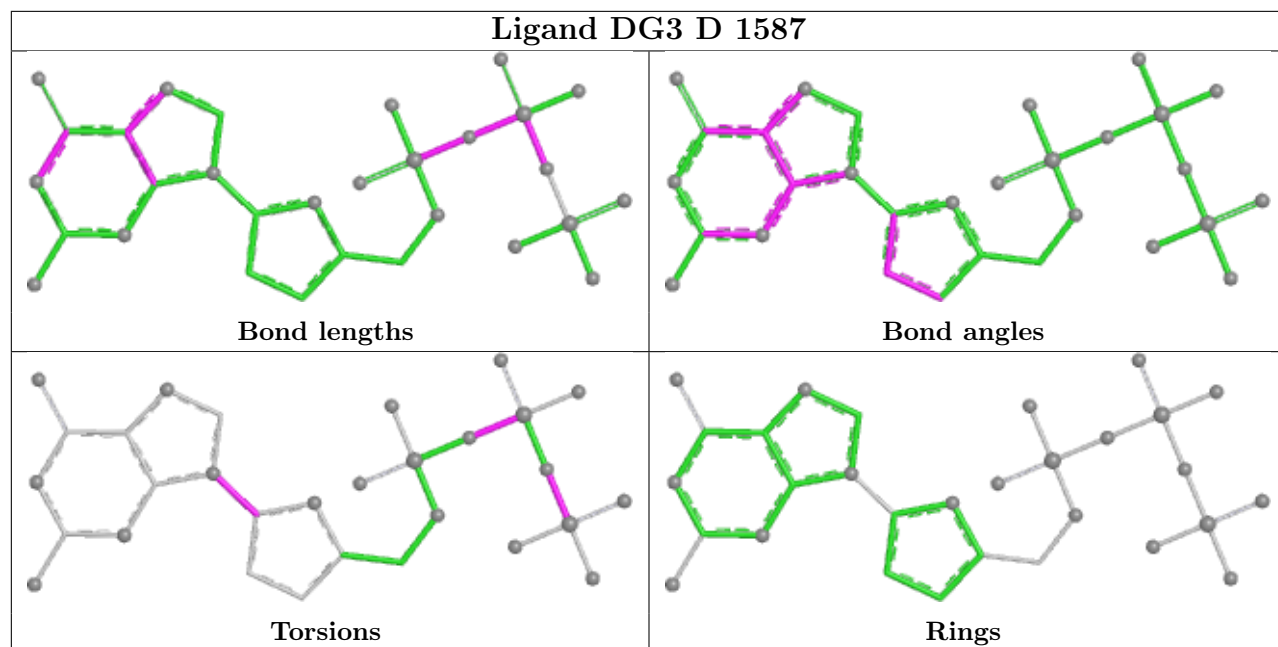


Ligand DG3 B 1584

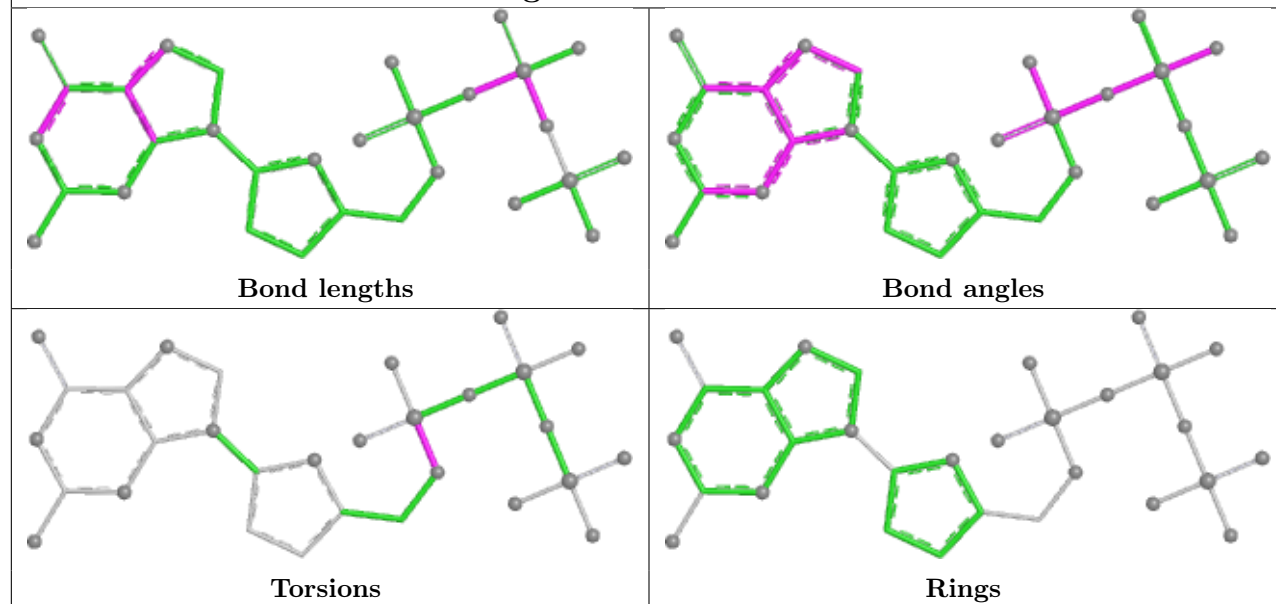


Ligand DG3 D 1586

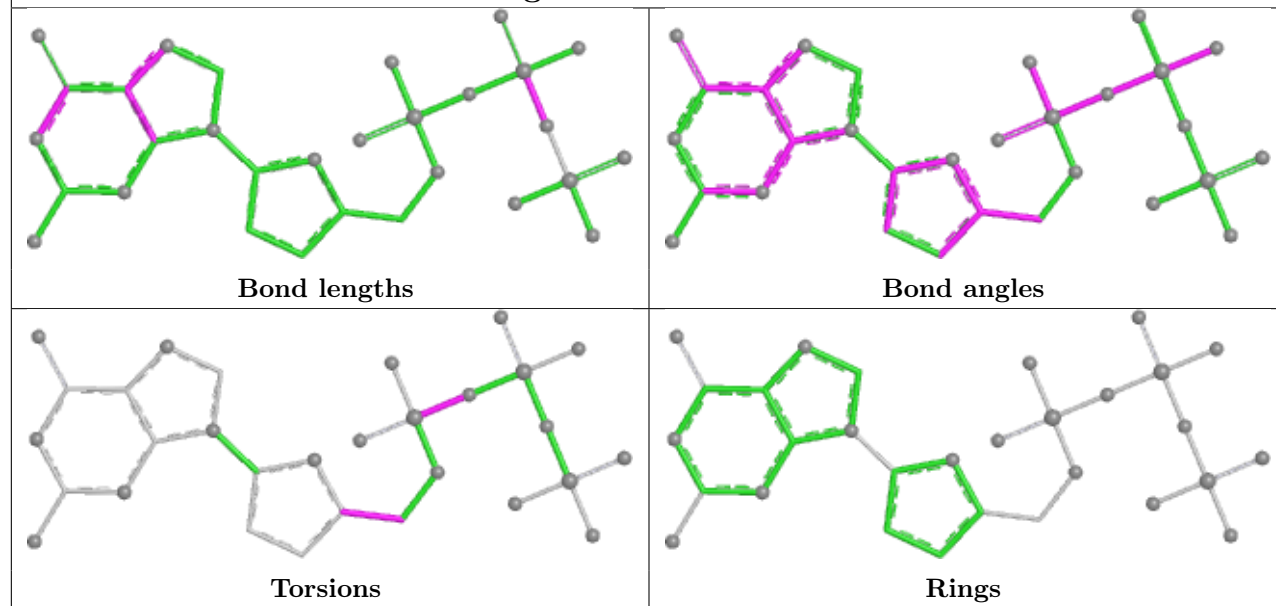


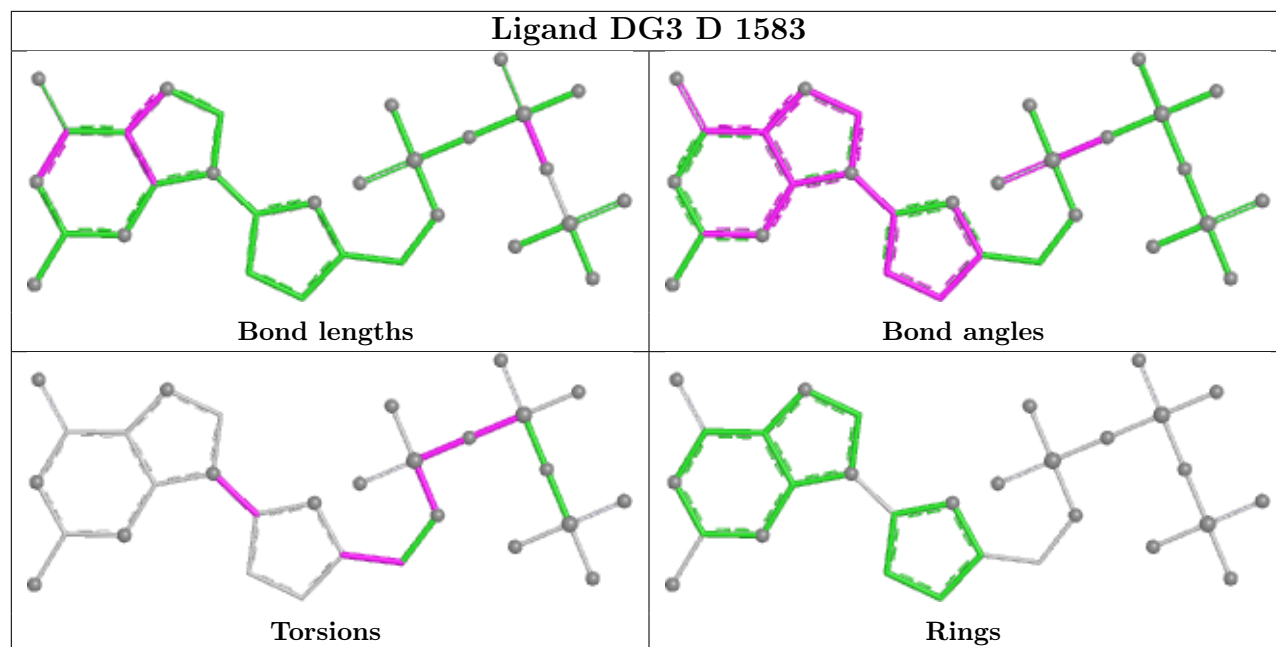


Ligand DG3 A 1585



Ligand DG3 C 1585





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	457/491 (93%)	-0.12	6 (1%) 75 75	31, 60, 108, 160	1 (0%)
1	B	443/491 (90%)	-0.15	6 (1%) 73 74	28, 58, 109, 152	0
1	C	457/491 (93%)	-0.08	11 (2%) 59 61	34, 63, 107, 133	0
1	D	442/491 (90%)	-0.19	10 (2%) 61 62	28, 57, 106, 142	1 (0%)
All	All	1799/1964 (91%)	-0.13	33 (1%) 67 68	28, 60, 108, 160	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	506	ASP	3.9
1	A	276	LEU	3.4
1	D	284	LEU	3.4
1	C	532	ILE	3.2
1	D	512	LYS	3.1
1	D	113	PRO	2.9
1	A	545	PHE	2.8
1	C	545	PHE	2.8
1	D	263	GLU	2.7
1	B	463	THR	2.6
1	A	282	ASP	2.6
1	C	510	GLN	2.6
1	C	284	LEU	2.5
1	C	538	SER	2.5
1	D	341	CYS	2.5
1	B	527	ASN	2.5
1	C	547	GLU	2.4
1	C	488	LEU	2.4
1	D	513	ASN	2.4
1	B	308	ILE	2.3
1	A	345	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	276	LEU	2.2
1	C	515	ILE	2.2
1	D	528	ARG	2.2
1	A	544	LYS	2.2
1	C	489	LEU	2.1
1	C	466	ILE	2.1
1	B	513	ASN	2.0
1	D	276	LEU	2.0
1	D	262	GLU	2.0
1	D	515	ILE	2.0
1	B	276	LEU	2.0
1	A	485	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

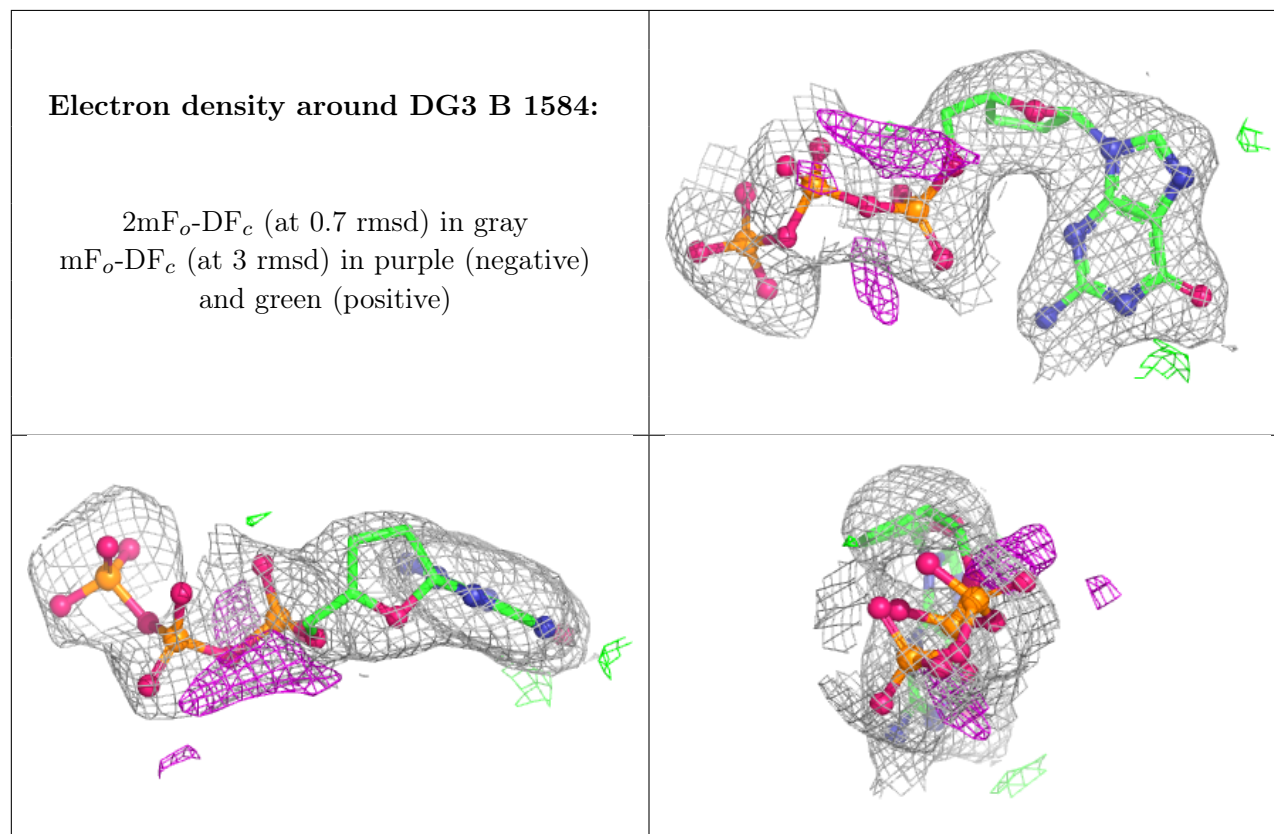
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	D	1588	5/5	0.69	0.12	135,137,138,140	0
4	SO4	A	1586	5/5	0.73	0.11	135,137,138,139	0
4	SO4	B	1589	5/5	0.74	0.10	139,141,141,142	0
4	SO4	D	1589	5/5	0.79	0.12	143,145,145,148	0
5	MG	B	1585	1/1	0.79	0.12	84,84,84,84	0
5	MG	B	1590	1/1	0.89	0.09	74,74,74,74	0
3	DG3	B	1584	30/30	0.92	0.09	39,58,108,215	0
3	DG3	B	1588	30/30	0.92	0.09	49,63,144,311	0
3	DG3	D	1587	30/30	0.93	0.09	53,65,161,351	0
3	DG3	D	1583	30/30	0.94	0.08	47,57,150,179	0
3	DG3	B	1587	30/30	0.94	0.10	49,81,119,164	0

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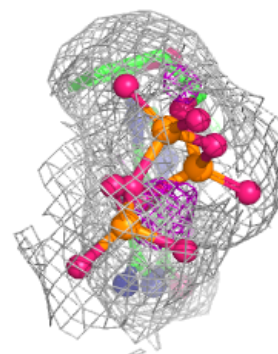
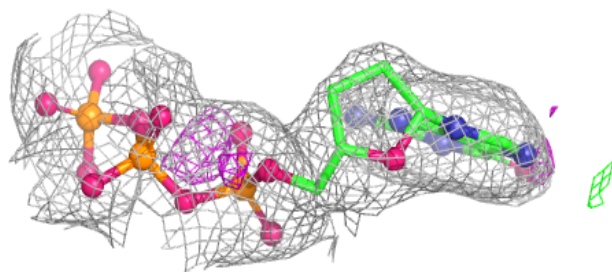
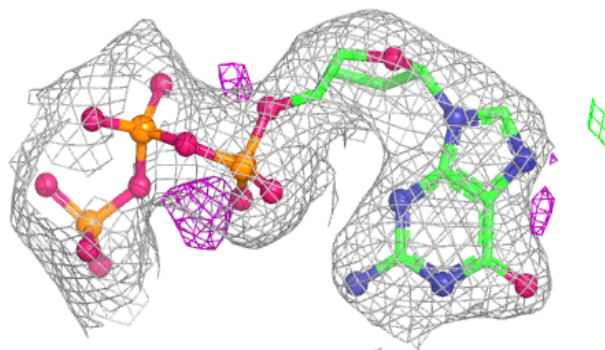
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	D	1584	1/1	0.94	0.08	85,85,85,85	0
3	DG3	D	1586	30/30	0.95	0.10	48,76,99,262	0
3	DG3	C	1585	30/30	0.95	0.09	48,66,120,265	0
3	DG3	A	1585	30/30	0.95	0.08	47,68,104,111	0
5	MG	D	1590	1/1	0.96	0.05	84,84,84,84	0
2	FE	A	1584	1/1	1.00	0.10	48,48,48,48	0
2	FE	B	1586	1/1	1.00	0.09	42,42,42,42	0
2	FE	C	1584	1/1	1.00	0.08	51,51,51,51	0
2	FE	D	1585	1/1	1.00	0.06	39,39,39,39	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.

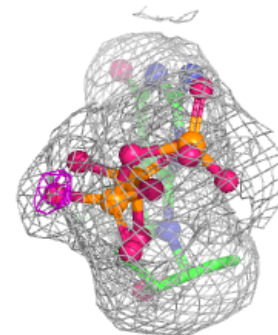
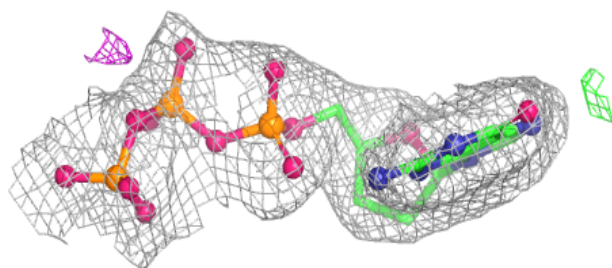
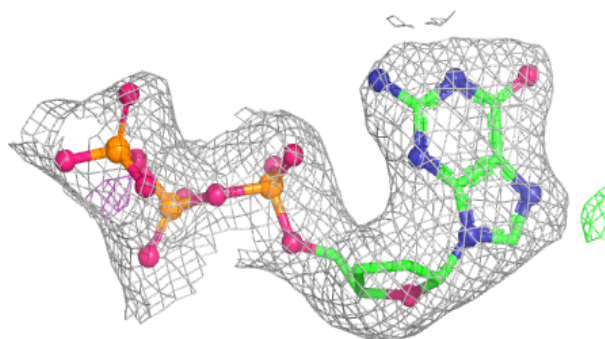


Electron density around DG3 B 1588:

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

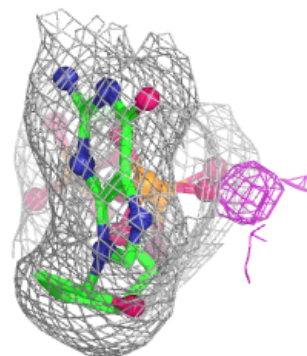
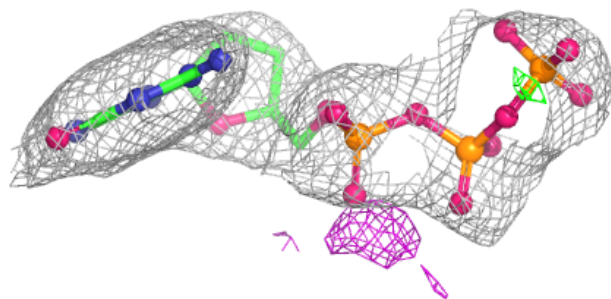
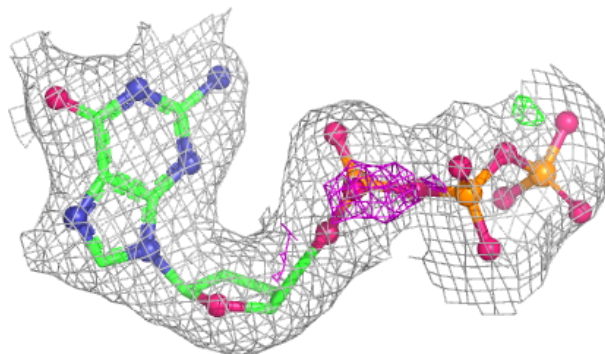
**Electron density around DG3 D 1587:**

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

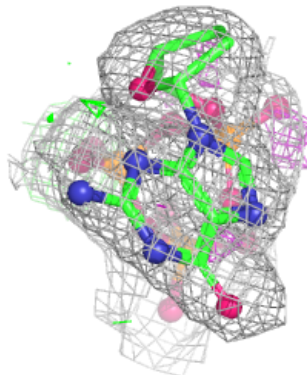
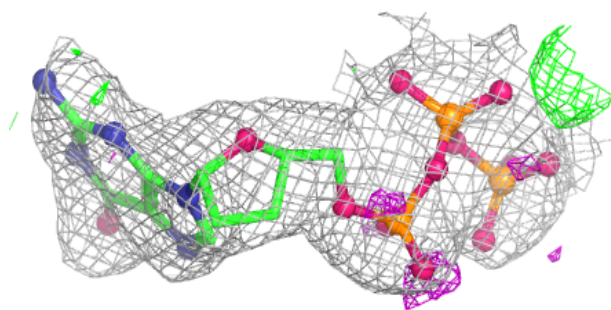
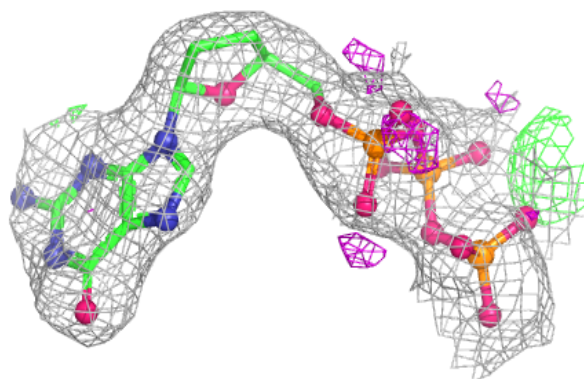


Electron density around DG3 D 1583:

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

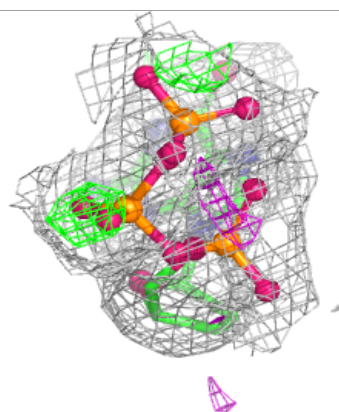
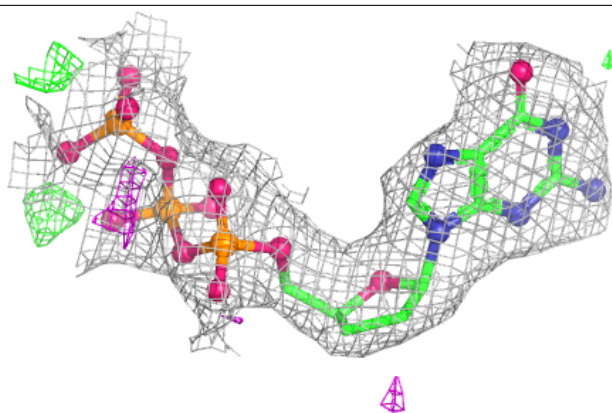
**Electron density around DG3 B 1587:**

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

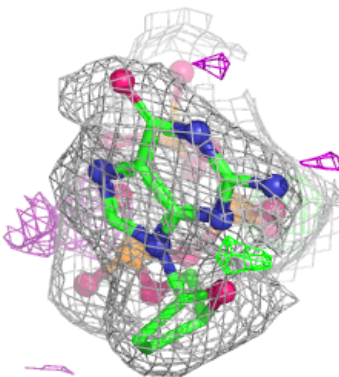
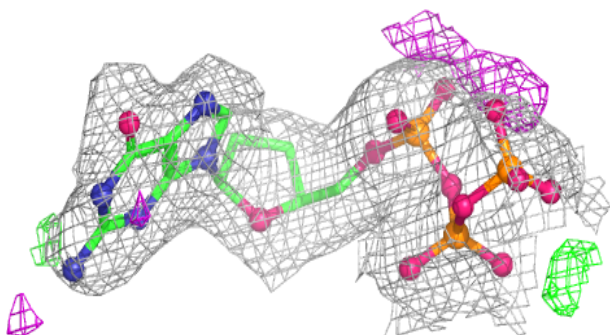
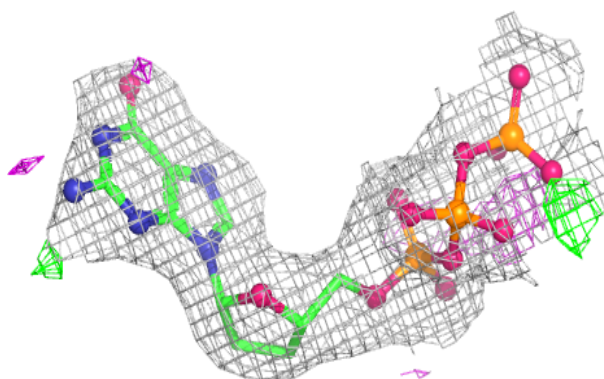


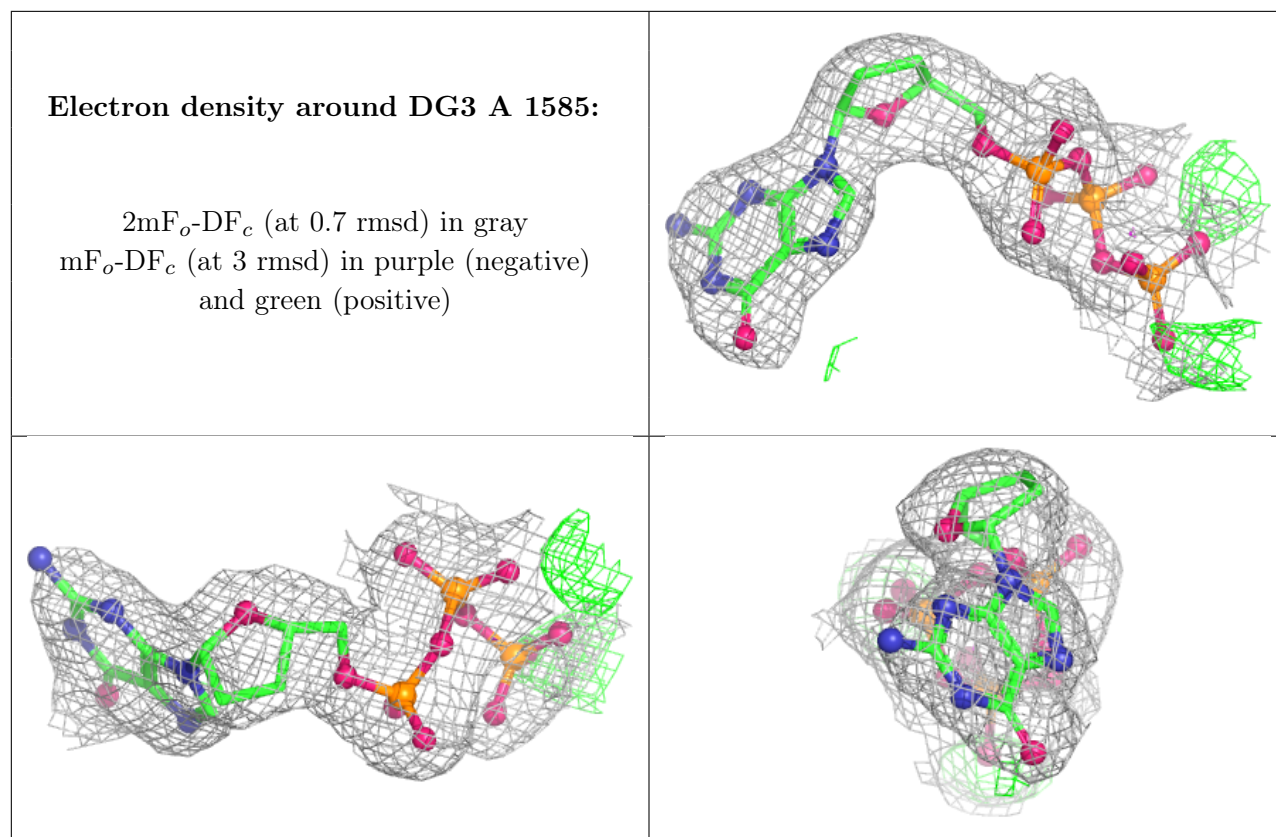
Electron density around DG3 D 1586:

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

**Electron density around DG3 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.