



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 08:47 pm BST

PDB ID : 1OT3
Title : Crystal structure of Drosophila deoxyribonucleotide kinase complexed with the substrate deoxythymidine
Authors : Mikkelsen, N.E.; Johansson, K.; Karlsson, A.; Knecht, W.; Andersen, G.; Piskur, J.; Munch-Petersen, B.; Eklund, H.
Deposited on : 2003-03-21
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

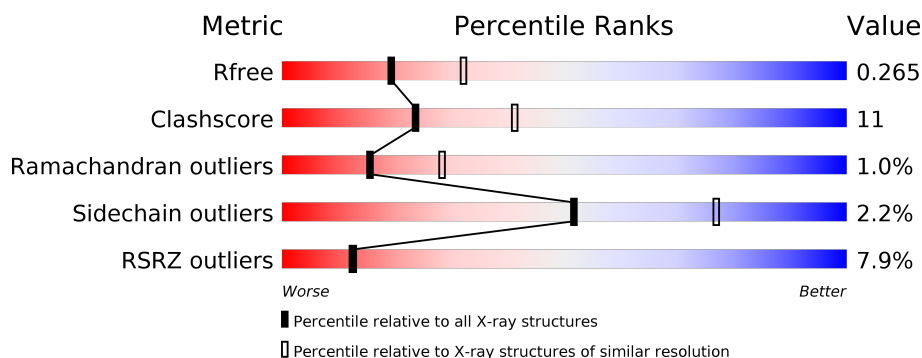
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	250	<div> <div>2%</div> <div> <div>57%</div> <div>21%</div> <div>•</div> <div>21%</div> </div> </div>
1	B	250	<div> <div>9%</div> <div> <div>59%</div> <div>16%</div> <div>•</div> <div>23%</div> </div> </div>
1	C	250	<div> <div>6%</div> <div> <div>59%</div> <div>18%</div> <div>•</div> <div>21%</div> </div> </div>
1	D	250	<div> <div>8%</div> <div> <div>56%</div> <div>20%</div> <div>•</div> <div>24%</div> </div> </div>
1	E	250	<div> <div>4%</div> <div> <div>56%</div> <div>19%</div> <div>•</div> <div>23%</div> </div> </div>
1	F	250	<div> <div>13%</div> <div> <div>58%</div> <div>18%</div> <div>•</div> <div>23%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	250	<div><div><div></div><div></div><div></div><div></div></div><div>7%56%19%•23%</div></div>
1	H	250	<div><div><div></div><div></div><div></div><div></div></div><div>%62%14%•23%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13338 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 Deoxyribonucleoside Kinase.

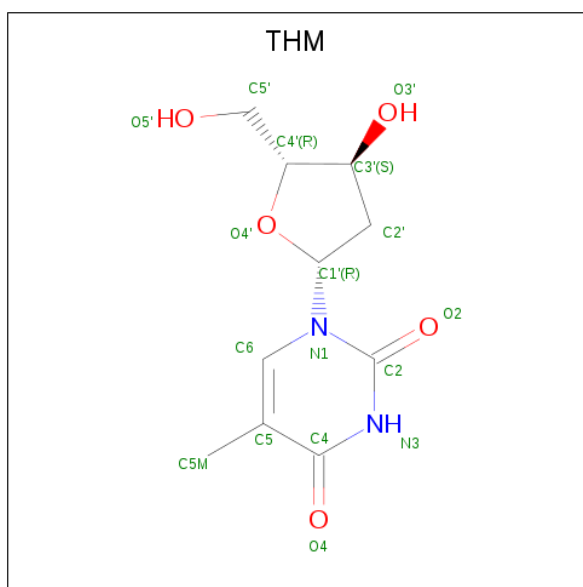
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	B	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	C	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	D	191	Total	C	N	O	S	0	0	0
			1587	1016	268	293	10			
1	E	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	F	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	G	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	H	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is THYMIDINE (three-letter code: THM) (formula: C₁₀H₁₄N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	10	2	5		
3	B	1	Total	C	N	O	0	0
			17	10	2	5		
3	C	1	Total	C	N	O	0	0
			17	10	2	5		
3	D	1	Total	C	N	O	0	0
			17	10	2	5		
3	E	1	Total	C	N	O	0	0
			17	10	2	5		
3	F	1	Total	C	N	O	0	0
			17	10	2	5		
3	G	1	Total	C	N	O	0	0
			17	10	2	5		
3	H	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	30	Total	O	0	0
			30	30		
4	C	25	Total	O	0	0
			25	25		
4	D	17	Total	O	0	0
			17	17		

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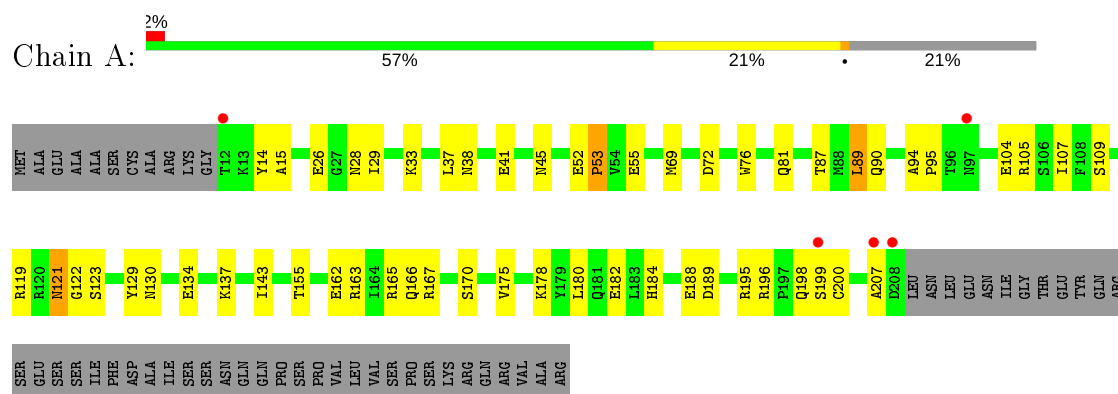
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	27	Total 27	O 27	0	0
4	F	16	Total 16	O 16	0	0
4	G	18	Total 18	O 18	0	0
4	H	65	Total 65	O 65	0	0

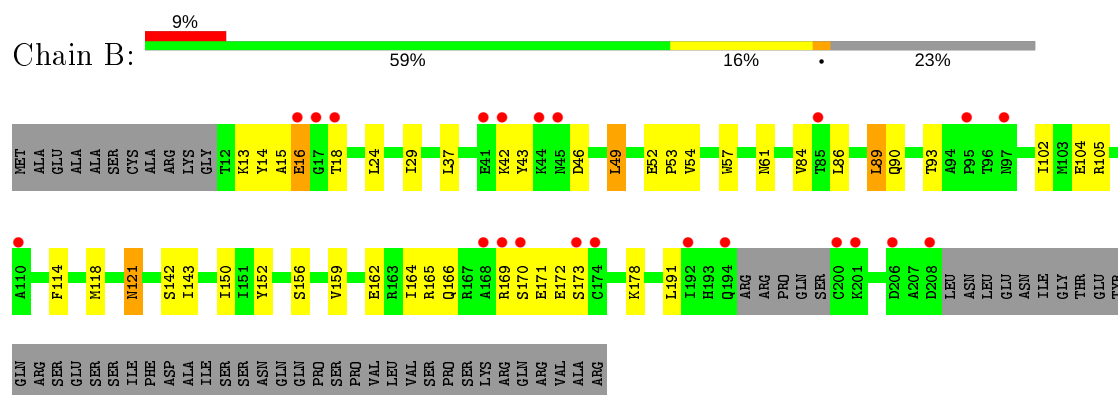
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

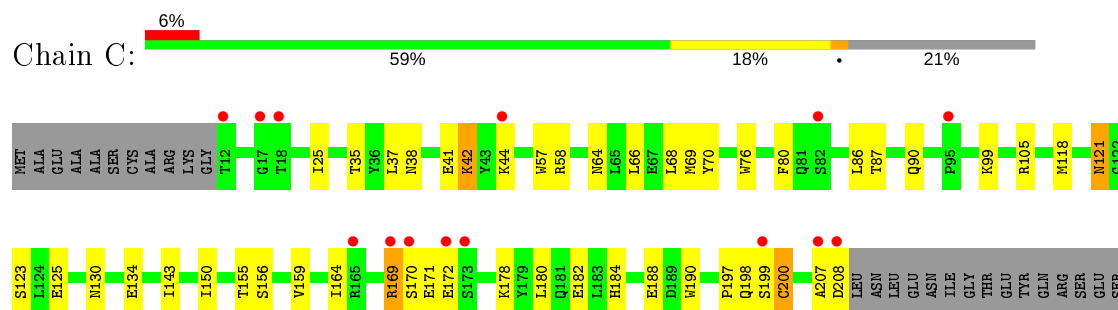
• Molecule 1: Deoxyribonucleoside Kinase



• Molecule 1: Deoxyribonucleoside Kinase



• Molecule 1: Deoxyribonucleoside Kinase



SER
ILE
PHE
ASP
ALA
ILE
SER
ASN
GLN
GLY
PRO
SER
PRO
VAL
LEU
VAL
SER
PRO
SER
LYS
ARG
GLN
ARG
VAL
ALA
ARG

• Molecule 1: Deoxyribonucleoside Kinase

Chain D: 8% 56% 20% 24%

MET
ALA
GLU
LEU
PHE
ASP
ALA
ILE
SER
ASN
GLN
GLY
PRO
SER
PRO
VAL
LEU
VAL
SER
PRO
SER
LYS
ARG
GLN
ARG
VAL
ALA
ARG

T12
K13
Y14
A15
E16
G17
T18
Q19
P20
G27
S31
G32
K33
T34
L37
N38
E41
K44
N45
D46
L49
E52
P53
V60
N61
L65
K74
M78
P79
F80
Y83
V84
T85
L86
Q90

P95
T96
N97
R98
K99
L100
C101
M102
I103
E104
L105
S106
A110
F114
V115
M118
M121
G122
S123
L124
F125
Q126
M130
H144
Y152
T155
S156
V159
R165
A168
R169
E172
S173
C174
V175
L191
I192
H193
GLN
ARG
PRO
GLN
SER
C200
K201

D208
LEU
ASN
LEU
GLU
ALA
SER
ILE
GLY
THR
TYR
GLN
ARG
SER
GLU
SER
PHE
ASP
ALA
ILE
SER
SER
ASN
GLN
GLY
PRO
SER
PRO
VAL
VAL
SER
PRO
SER
LYS
ARG
GLN
ARG
VAL
ALA
ARG

• Molecule 1: Deoxyribonucleoside Kinase

Chain E: 4% 56% 19% 23%

MET
ALA
GLU
LEU
PHE
ASP
ALA
ILE
SER
ASN
GLN
GLY
PRO
SER
PRO
VAL
LEU
VAL
SER
PRO
SER
LYS
ARG
GLN
ARG
VAL
ALA
ARG

T12
G17
T18
L24
I25
N28
K33
L37
N38
H39
K42
I47
C48
L49
E52
P53
V60
L65
L66
E67
Y70
K71
D72
K75
L86
L89
Q90
S91
H92
N97
L100
E104

R105
M118
R119
R120
M121
G122
S123
Y129
I139
V145
I150
I151
Y152
T155
E158
I164
Q166
R167
A168
R169
S170
E171
E172
S173
C174
V175
P176
L177
K178
I179
L180
Q181
E182
D189
M190
L191
Q194
ARG
PRO
GLN
SER
C200
A207
D208
LEU
ASN
LEU

GLU
ASN
ILE
GLY
THR
GLU
TYR
GLN
ARG
SER
GLU
SER
SER
ILE
PHE
ASP
ALA
ILE
SER
SER
ASN
GLN
GLY
PRO
PRO
VAL
LEU
VAL
SER
PRO
LYS
SER
ARG
GLN
ARG
VAL
ALA
ARG

• Molecule 1: Deoxyribonucleoside Kinase

Chain F: 13% 58% 18% 23%

MET
ALA
GLU
LEU
PHE
ASP
ALA
ILE
SER
ASN
GLN
GLY
PRO
SER
PRO
VAL
LEU
VAL
SER
PRO
SER
LYS
ARG
GLN
ARG
VAL
ALA
ARG

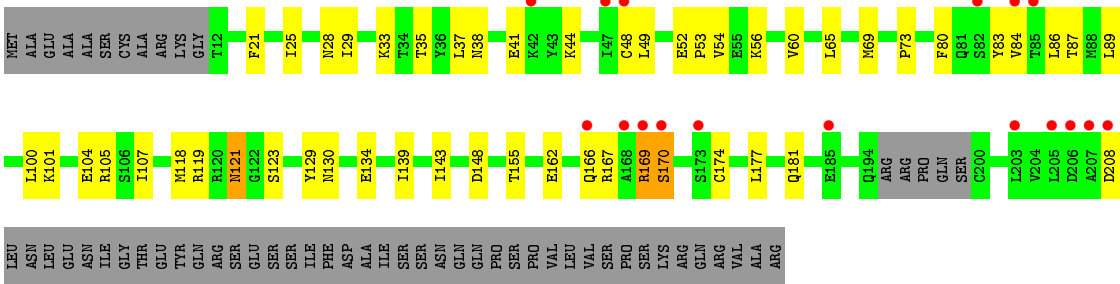
T12
G17
T18
P20
F21
I25
E26
G27
N28
I29
G30
S31
L37
K42
E52
P53
V54
E55
K56
W57
R58
N64
E67
L68
M69
K74
S82
Y83
V84
L89
H92
T93
A94
P95
T96
N97
K98

K99
L100
M103
E104
R105
S106
F107
F108
M117
M121
G122
S123
E125
M128
Y129
M130
E134
W135
I139
I143
P144
V145
L153
R154
T155
S156
V159
A160
I164
R165
Q166
R167
A168
R169
S170
S173
C174
K178
E182
L186
H193
Q194
ARG
ARG

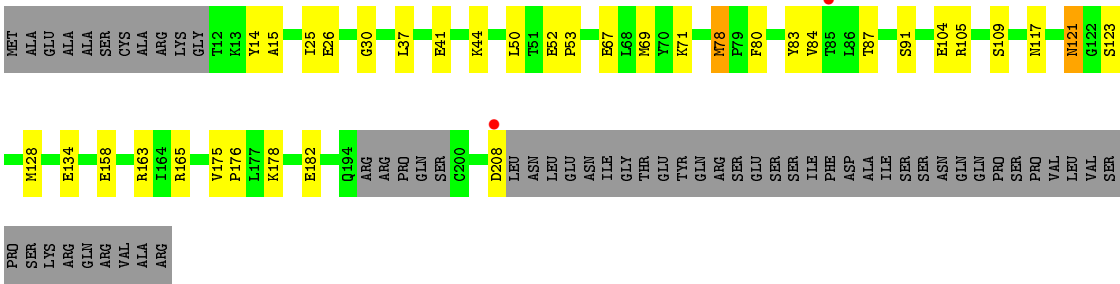
PRO
GLN
SER
C200
K201
V202
L203
A207
D208
LEU
ASN
LEU
GLU
ASN
ILE
GLY
THR
GLU
TYR
GLN
ARG
SER
SER
ILE
PHE
ASP
ALA
ILE
SER
SER
ASN
GLN
GLY
PRO
PRO
VAL
LEU
VAL
SER
PRO
SER
LYS
ARG
GLN
ARG
VAL
VAL
ALA
ARG

• Molecule 1: Deoxyribonucleoside Kinase

Chain G: 7% 56% 19% 23%



• Molecule 1: Deoxyribonucleoside Kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.38 Å 71.16 Å 226.27 Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (25.00-2.50) 89.9 (24.89-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.50 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.276 0.219 , 0.265	Depositor DCC
R_{free} test set	3560 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.004 for k,h,-l 0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13338	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.69% 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: THM, 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	0.47	0/1678	0.64	0/2268
1	B	0.35	0/1632	0.52	0/2205
1	C	0.33	0/1678	0.50	0/2268
1	D	0.32	0/1623	0.48	0/2193
1	E	0.33	0/1632	0.49	0/2205
1	F	0.30	0/1632	0.46	0/2205
1	G	0.33	0/1632	0.48	0/2205
1	H	0.47	0/1632	0.60	0/2205
All	All	0.37	0/13139	0.52	0/17754

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1640	0	1629	43	0
1	B	1596	0	1582	34	0
1	C	1640	0	1629	41	0
1	D	1587	0	1574	41	0
1	E	1596	0	1582	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1596	0	1582	35	0
1	G	1596	0	1582	35	0
1	H	1596	0	1582	25	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	17	0	13	0	0
3	B	17	0	14	0	0
3	C	17	0	13	1	0
3	D	17	0	13	1	0
3	E	17	0	13	0	0
3	F	17	0	13	0	0
3	G	17	0	13	0	0
3	H	17	0	14	0	0
4	A	112	0	0	5	0
4	B	30	0	0	1	0
4	C	25	0	0	0	0
4	D	17	0	0	1	0
4	E	27	0	0	1	0
4	F	16	0	0	1	0
4	G	18	0	0	1	0
4	H	65	0	0	2	0
All	All	13338	0	12848	289	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 289 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:G:25:ILE:HG13	1:G:37:LEU:HD21	1.38	1.05
1:H:37:LEU:HD11	1:H:104:GLU:HB2	1.51	0.92
1:F:125:GLU:H	1:F:128:MET:HE3	1.41	0.85
1:D:165:ARG:HA	1:D:165:ARG:HH11	1.47	0.80
1:D:19:GLN:HE22	1:D:101:LYS:NZ	1.81	0.79

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	195/250 (78%)	184 (94%)	10 (5%)	1 (0%)	29	48
1	B	188/250 (75%)	158 (84%)	29 (15%)	1 (0%)	29	48
1	C	195/250 (78%)	177 (91%)	17 (9%)	1 (0%)	29	48
1	D	187/250 (75%)	168 (90%)	15 (8%)	4 (2%)	7	11
1	E	188/250 (75%)	171 (91%)	16 (8%)	1 (0%)	29	48
1	F	188/250 (75%)	170 (90%)	14 (7%)	4 (2%)	7	11
1	G	188/250 (75%)	157 (84%)	28 (15%)	3 (2%)	9	17
1	H	188/250 (75%)	173 (92%)	15 (8%)	0	100	100
All	All	1517/2000 (76%)	1358 (90%)	144 (10%)	15 (1%)	15	28

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	174	CYS
1	B	16	GLU
1	D	173	SER
1	E	174	CYS
1	F	20	PRO

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	182/227 (80%)	176 (97%)	6 (3%)	38	64
1	B	177/227 (78%)	170 (96%)	7 (4%)	31	56
1	C	182/227 (80%)	177 (97%)	5 (3%)	44	71
1	D	176/227 (78%)	175 (99%)	1 (1%)	86	95
1	E	177/227 (78%)	174 (98%)	3 (2%)	60	82
1	F	177/227 (78%)	173 (98%)	4 (2%)	50	76
1	G	177/227 (78%)	175 (99%)	2 (1%)	73	89
1	H	177/227 (78%)	173 (98%)	4 (2%)	50	76
All	All	1425/1816 (78%)	1393 (98%)	32 (2%)	52	77

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	121	ASN
1	C	200	CYS
1	H	121	ASN
1	C	169	ARG
1	D	61	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	61	ASN
1	E	117	ASN
1	G	121	ASN
1	D	117	ASN
1	D	130	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	THM	E	1402	-	15,18,18	1.55	3 (20%)	16,26,26	2.89	10 (62%)
3	THM	H	1407	-	15,18,18	1.79	5 (33%)	16,26,26	2.94	9 (56%)
2	SO4	E	1302	-	4,4,4	0.33	0	6,6,6	0.08	0
3	THM	G	1403	-	15,18,18	1.54	2 (13%)	16,26,26	2.94	9 (56%)
3	THM	A	1400	-	15,18,18	1.64	3 (20%)	16,26,26	2.92	9 (56%)
2	SO4	G	1303	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	D	1301	-	4,4,4	0.28	0	6,6,6	0.10	0
3	THM	B	1406	-	15,18,18	1.46	2 (13%)	16,26,26	2.83	9 (56%)
2	SO4	A	1300	-	4,4,4	0.33	0	6,6,6	0.15	0
2	SO4	F	1304	-	4,4,4	0.19	0	6,6,6	0.06	0
3	THM	D	1401	-	15,18,18	1.47	2 (13%)	16,26,26	2.90	9 (56%)
3	THM	C	1405	-	15,18,18	1.48	2 (13%)	16,26,26	2.80	9 (56%)
3	THM	F	1404	-	15,18,18	1.52	3 (20%)	16,26,26	2.82	9 (56%)
2	SO4	A	1308	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	C	1305	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	H	1307	-	4,4,4	0.18	0	6,6,6	0.27	0
2	SO4	B	1306	-	4,4,4	0.21	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THM	E	1402	-	-	3/3/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THM	G	1403	-	-	2/3/18/18	0/2/2/2
3	THM	A	1400	-	-	3/3/18/18	0/2/2/2
3	THM	B	1406	-	-	3/3/18/18	0/2/2/2
3	THM	H	1407	-	-	3/3/18/18	0/2/2/2
3	THM	D	1401	-	-	3/3/18/18	0/2/2/2
3	THM	C	1405	-	-	3/3/18/18	0/2/2/2
3	THM	F	1404	-	-	3/3/18/18	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1403	THM	O3'-C3'	4.09	1.52	1.43
3	A	1400	THM	O3'-C3'	3.84	1.51	1.43
3	E	1402	THM	O3'-C3'	3.81	1.51	1.43
3	F	1404	THM	O3'-C3'	3.67	1.51	1.43
3	C	1405	THM	O3'-C3'	3.60	1.51	1.43

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1400	THM	C4-N3-C2	5.91	120.14	115.14
3	C	1405	THM	C4-N3-C2	5.74	119.99	115.14
3	B	1406	THM	C4-N3-C2	5.68	119.94	115.14
3	D	1401	THM	C4-N3-C2	5.66	119.92	115.14
3	E	1402	THM	C4-N3-C2	5.64	119.90	115.14

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1402	THM	C3'-C4'-C5'-O5'
3	E	1402	THM	O4'-C1'-N1-C6
3	H	1407	THM	O4'-C4'-C5'-O5'
3	H	1407	THM	C3'-C4'-C5'-O5'
3	H	1407	THM	O4'-C1'-N1-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1401	THM	1	0
3	C	1405	THM	1	0

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	197/250 (78%)	-0.02	5 (2%) 57 61	20, 37, 59, 97	0
1	B	192/250 (76%)	0.47	22 (11%) 4 4	28, 57, 98, 110	0
1	C	197/250 (78%)	0.43	14 (7%) 16 16	36, 65, 106, 115	0
1	D	191/250 (76%)	0.60	20 (10%) 6 6	41, 72, 103, 114	0
1	E	192/250 (76%)	0.33	9 (4%) 31 33	36, 61, 95, 110	0
1	F	192/250 (76%)	0.92	33 (17%) 1 1	42, 79, 107, 116	0
1	G	192/250 (76%)	0.61	17 (8%) 9 9	32, 69, 108, 123	0
1	H	192/250 (76%)	-0.18	2 (1%) 82 84	21, 35, 55, 71	0
All	All	1545/2000 (77%)	0.39	122 (7%) 12 12	20, 60, 103, 123	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	THR	7.7
1	F	168	ALA	5.4
1	F	95	PRO	5.0
1	F	170	SER	5.0
1	G	206	ASP	4.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
3	THM	C	1405	17/17	0.92	0.27	55,58,64,65	0
3	THM	G	1403	17/17	0.94	0.28	66,70,72,73	0
2	SO4	D	1301	5/5	0.95	0.15	55,56,60,61	0
3	THM	B	1406	17/17	0.96	0.23	29,37,45,45	0
3	THM	D	1401	17/17	0.96	0.26	48,51,58,60	0
2	SO4	F	1304	5/5	0.96	0.16	65,67,68,70	0
3	THM	E	1402	17/17	0.96	0.19	39,44,52,52	0
3	THM	F	1404	17/17	0.96	0.20	45,49,56,58	0
3	THM	A	1400	17/17	0.97	0.20	27,31,36,38	0
2	SO4	G	1303	5/5	0.97	0.12	69,69,69,72	0
3	THM	H	1407	17/17	0.98	0.18	16,26,30,31	0
2	SO4	C	1305	5/5	0.98	0.11	66,67,68,69	0
2	SO4	A	1300	5/5	0.99	0.09	29,29,33,35	0
2	SO4	E	1302	5/5	0.99	0.12	49,49,51,52	0
2	SO4	A	1308	5/5	0.99	0.19	43,46,49,50	0
2	SO4	H	1307	5/5	0.99	0.14	30,31,33,34	0
2	SO4	B	1306	5/5	0.99	0.12	43,44,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.