



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:26 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

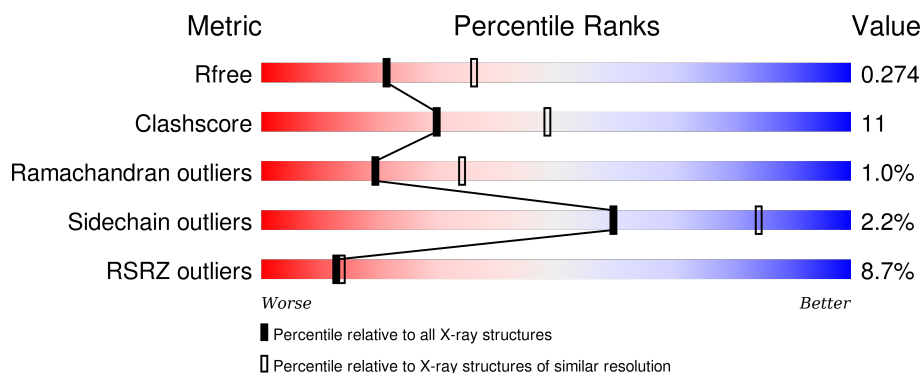
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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>57% 21% • 21%</div> </div>
1	B	250	<div> <div>10%</div> <div>59% 16% • 23%</div> </div>
1	C	250	<div> <div>7%</div> <div>59% 18% • 21%</div> </div>
1	D	250	<div> <div>9%</div> <div>56% 20% • 24%</div> </div>
1	E	250	<div> <div>4%</div> <div>56% 19% • 23%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	250	<div><div></div><div>14%</div><div>58%</div><div>18%</div><div>•</div><div>23%</div></div>
1	G	250	<div><div></div><div>7%</div><div>56%</div><div>19%</div><div>•</div><div>23%</div></div>
1	H	250	<div><div></div><div>%</div><div>62%</div><div>14%</div><div>•</div><div>23%</div></div>

2 Entry composition

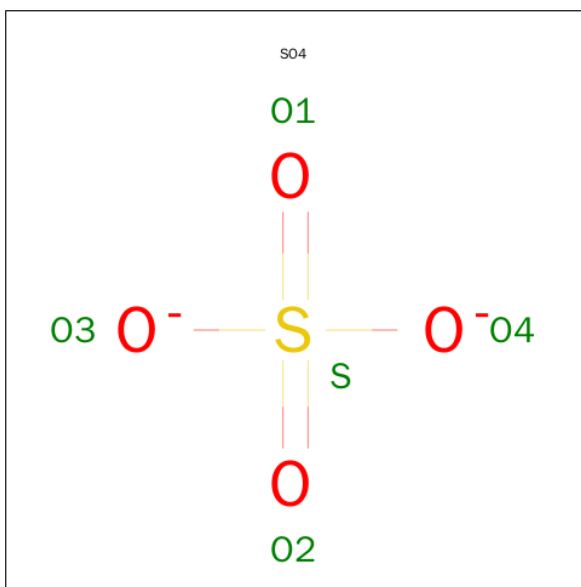
There are 4 unique types of molecules in this entry. The entry contains 13338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

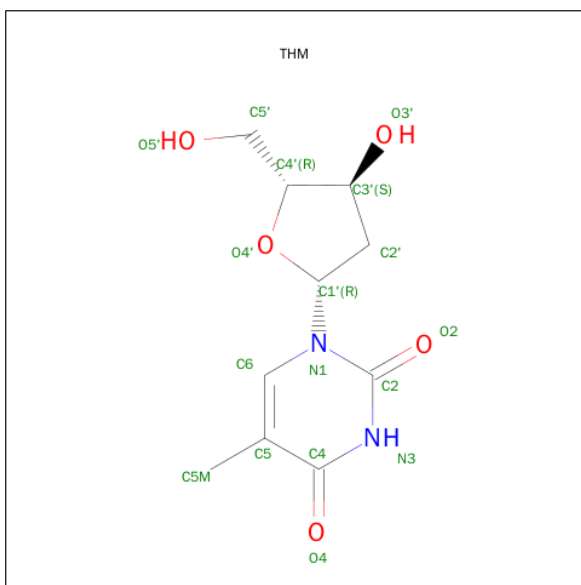
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	B	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	C	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	D	191	Total	C	N	O	S	0	0	0
			1587	1016	268	293	10			
1	E	192	Total	C	N	O	S	0	0	0
			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	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	A	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	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	G	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	C	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	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		

Continued on next page...

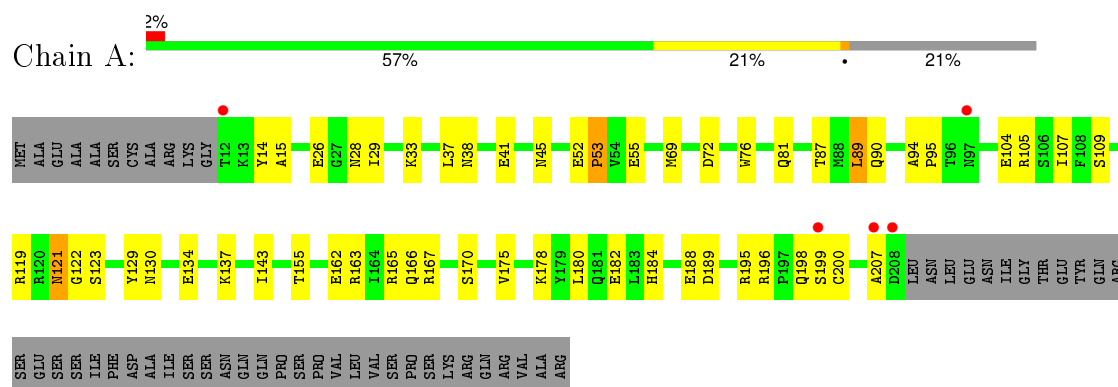
Continued from previous page...

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

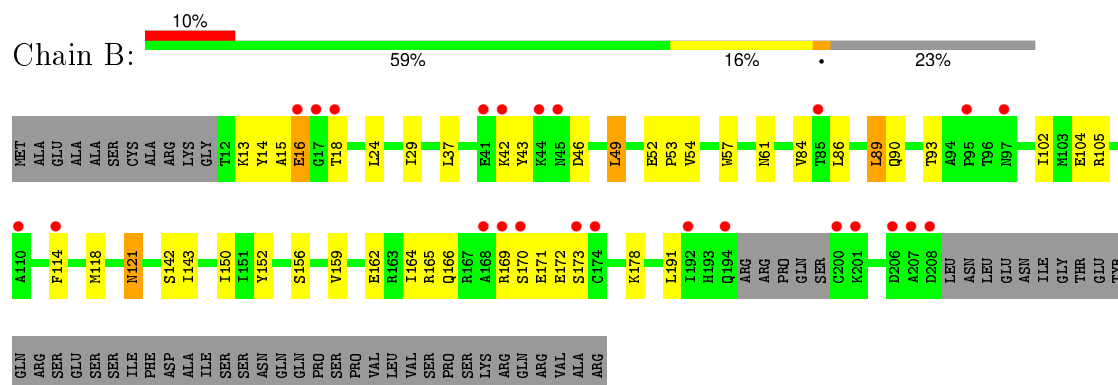
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

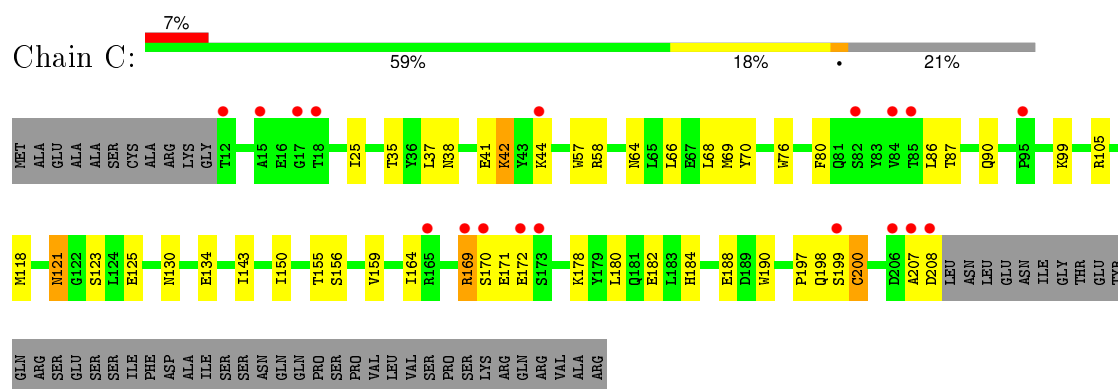
• Molecule 1: Deoxyribonucleoside Kinase



• Molecule 1: Deoxyribonucleoside Kinase



• Molecule 1: Deoxyribonucleoside Kinase



Chain D:

9% 56% 20% 24%

MET ALA GLU ALA ALA SER CYS ALA ARG LYS GLY T12 K13 Y14 A15 E16 G17 T18 Q19 P20 G27 S31 G32 K33 T34 L37 N38 E41 K44 M45 D46 L49 E52 P53 V60 N61 L65 K74 M78 P79 F80 Y83 V84 T85 L86 Q90 P96 T96 M97 K98 L100 K101 I102 M103 E104 R105 S106 A110 F114 Y115 M118 N121 G122 S123 L124 E125 Q126 N130 H144 Y152 T155 S156 V159 R165 A168 R169 E172 S173 C174 V175 L191 I192 H193 G194 ARG ARG PRO GLN SER C200 K201

Chain E:

Category	Percentage
Green	56%
Yellow	19%
Red	4%
Grey	23%

Residue list (top to bottom): MET, ALA, GLU, ALA, ALA, SER, CYS, ALA, ARG, LYS, GLY, T12, T18, L24, T28, K33, L37, N38, H39, K42, I47, C48, L49, E52, P63, V60, L65, L66, E67, Y70, K71, D72, K75, L86, L89, Q90, S91, H92, N97, L100, F104, R105, M18, R119, R120, N121, G122, S123, Y129, I139, E140, E141, V145, I150, I151, Y152, T155, E158, I164, R165, Q166, R167, A168, R169, S170, E171, E172, S173, C174, V175, P176, L177, K178, Y179, L180, Q181, E182, D189, H190, L191, Q194, A194, ARG, ARG, PRO, GLN, SER, C200, A207, D208, F209.

Chain F:

14% 58% 18% 23%

Residue	Count	Category
MET	1	Category 1 (14%)
ALA	1	Category 1 (14%)
GLU	1	Category 1 (14%)
ALA	1	Category 1 (14%)
SER	1	Category 1 (14%)
CYS	1	Category 1 (14%)
ALA	1	Category 1 (14%)
ARG	1	Category 1 (14%)
LYS	1	Category 1 (14%)
GLY	1	Category 1 (14%)
T12	1	Category 2 (58%)
G17	1	Category 2 (58%)
T18	1	Category 2 (58%)
Q19	1	Category 2 (58%)
P20	1	Category 2 (58%)
F21	1	Category 2 (58%)
I25	1	Category 2 (58%)
E26	1	Category 2 (58%)
G27	1	Category 2 (58%)
N28	1	Category 2 (58%)
I29	1	Category 2 (58%)
G30	1	Category 2 (58%)
S31	1	Category 2 (58%)
L37	1	Category 2 (58%)
R42	1	Category 2 (58%)
T43	1	Category 2 (58%)
E52	1	Category 2 (58%)
P53	1	Category 2 (58%)
V54	1	Category 2 (58%)
E55	1	Category 2 (58%)
R56	1	Category 2 (58%)
N57	1	Category 2 (58%)
R58	1	Category 2 (58%)
N64	1	Category 2 (58%)
E67	1	Category 2 (58%)
L68	1	Category 2 (58%)
M69	1	Category 2 (58%)
K74	1	Category 2 (58%)
S82	1	Category 2 (58%)
Y83	1	Category 2 (58%)
V84	1	Category 2 (58%)
L89	1	Category 2 (58%)
H92	1	Category 2 (58%)
T93	1	Category 2 (58%)
A94	1	Category 2 (58%)
P95	1	Category 2 (58%)
T96	1	Category 2 (58%)
N97	1	Category 2 (58%)
R98	1	Category 3 (18%)
R99	1	Category 3 (18%)
L100	1	Category 3 (18%)
M103	1	Category 3 (18%)
E104	1	Category 3 (18%)
R105	1	Category 3 (18%)
S106	1	Category 3 (18%)
I107	1	Category 3 (18%)
M108	1	Category 3 (18%)
N117	1	Category 3 (18%)
M121	1	Category 3 (18%)
G122	1	Category 3 (18%)
S123	1	Category 3 (18%)
I124	1	Category 3 (18%)
E125	1	Category 3 (18%)
M128	1	Category 3 (18%)
I129	1	Category 3 (18%)
N130	1	Category 3 (18%)
E134	1	Category 3 (18%)
M135	1	Category 3 (18%)
GLU	1	Category 3 (18%)
I139	1	Category 3 (18%)
I143	1	Category 3 (18%)
H144	1	Category 3 (18%)
V145	1	Category 3 (18%)
L153	1	Category 3 (18%)
R154	1	Category 3 (18%)
T155	1	Category 3 (18%)
S156	1	Category 3 (18%)
V159	1	Category 3 (18%)
GLN	1	Category 3 (18%)
A160	1	Category 3 (18%)
L164	1	Category 3 (18%)
R165	1	Category 3 (18%)
L166	1	Category 3 (18%)
R167	1	Category 3 (18%)
L168	1	Category 3 (18%)
R169	1	Category 3 (18%)
S170	1	Category 3 (18%)
S173	1	Category 3 (18%)
C174	1	Category 3 (18%)
K178	1	Category 3 (18%)
E182	1	Category 3 (18%)
L186	1	Category 3 (18%)
H193	1	Category 3 (18%)
Q194	1	Category 3 (18%)
A97	1	Category 3 (18%)
ARG	1	Category 4 (23%)
PRO	1	Category 4 (23%)
GLN	1	Category 4 (23%)
SER	1	Category 4 (23%)
C200	1	Category 4 (23%)
K201	1	Category 4 (23%)
V202	1	Category 4 (23%)
L203	1	Category 4 (23%)
V204	1	Category 4 (23%)
A207	1	Category 4 (23%)
E208	1	Category 4 (23%)
LEU	1	Category 4 (23%)
ASN	1	Category 4 (23%)
LEU	1	Category 4 (23%)
GLU	1	Category 4 (23%)
GLN	1	Category 4 (23%)
ARG	1	Category 4 (23%)
SER	1	Category 4 (23%)
GLU	1	Category 4 (23%)
SER	1	Category 4 (23%)
ILE	1	Category 4 (23%)
ILE	1	Category 4 (23%)
PHE	1	Category 4 (23%)
ASP	1	Category 4 (23%)
ALA	1	Category 4 (23%)
ILE	1	Category 4 (23%)
SER	1	Category 4 (23%)
SER	1	Category 4 (23%)
ASN	1	Category 4 (23%)
GLN	1	Category 4 (23%)
PRO	1	Category 4 (23%)
SER	1	Category 4 (23%)
PRO	1	Category 4 (23%)
VAL	1	Category 4 (23%)
LEU	1	Category 4 (23%)
VAL	1	Category 4 (23%)
SER	1	Category 4 (23%)
PRO	1	Category 4 (23%)
SER	1	Category 4 (23%)
LYS	1	Category 4 (23%)
ARG	1	Category 4 (23%)
GLN	1	Category 4 (23%)
ARG		

[illegible]

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	GLN	PRO	SER	PRO	VAL	LEU	VAL	SER	PRO	SER	SER	LYS	ARG	GLN	ARG	VAL	ALA	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: Deoxyribonucleoside Kinase



MET	ALA	GLU	ALA	ALA	SER	CYS	ALA	ARG	LYS	GLY	T12	K13	Y14	A15	I25	E26	G30	L37	E41	K44	L50	T51	E52	P63	E67	L68	M69	Y70	K71	M78	P79	F80	Y83	Y84	T85	L86	T87	S91	E104	R105	S109	N117	M121	G122	S123
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------

M128	E134	E158	R163	T164	R165	V175	P176	L177	K178	E182	G194	ARG	ARG	PRO	GLN	SER	C200	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	GLN	PRO	SER	PRO	VAL	LEU	VAL	SER
------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	SER	LYS	ARG	GLN	ARG	VAL	ALA	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----

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 0.225 , 0.274	Depositor DCC
R_{free} test set	3560 reflections (5.09%)	DCC
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 , 50.9	EDS
Estimated twinning fraction	0.000 for -k,-h,-l 0.004 for k,h,-l 0.023 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 70001 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

Continued on next page...

Continued from previous page...

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%)	34	55
1	B	188/250 (75%)	158 (84%)	29 (15%)	1 (0%)	34	55
1	C	195/250 (78%)	177 (91%)	17 (9%)	1 (0%)	34	55
1	D	187/250 (75%)	168 (90%)	15 (8%)	4 (2%)	9	14
1	E	188/250 (75%)	171 (91%)	16 (8%)	1 (0%)	34	55
1	F	188/250 (75%)	170 (90%)	14 (7%)	4 (2%)	9	14
1	G	188/250 (75%)	157 (84%)	28 (15%)	3 (2%)	12	21
1	H	188/250 (75%)	173 (92%)	15 (8%)	0	100	100
All	All	1517/2000 (76%)	1358 (90%)	144 (10%)	15 (1%)	19	34

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%)	45	73
1	B	177/227 (78%)	170 (96%)	7 (4%)	38	64
1	C	182/227 (80%)	177 (97%)	5 (3%)	52	79
1	D	176/227 (78%)	175 (99%)	1 (1%)	90	97
1	E	177/227 (78%)	174 (98%)	3 (2%)	68	89
1	F	177/227 (78%)	173 (98%)	4 (2%)	58	83
1	G	177/227 (78%)	175 (99%)	2 (1%)	80	94
1	H	177/227 (78%)	173 (98%)	4 (2%)	58	83
All	All	1425/1816 (78%)	1393 (98%)	32 (2%)	60	84

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	SO4	A	1300	-	4,4,4	0.43	0	6,6,6	0.29	0
2	SO4	A	1308	-	4,4,4	0.09	0	6,6,6	0.12	0
3	THM	A	1400	-	13,18,18	1.60	2 (15%)	16,26,26	2.90	9 (56%)
2	SO4	B	1306	-	4,4,4	0.18	0	6,6,6	0.07	0
3	THM	B	1406	-	13,18,18	1.46	2 (15%)	16,26,26	2.82	8 (50%)
2	SO4	C	1305	-	4,4,4	0.20	0	6,6,6	0.08	0
3	THM	C	1405	-	13,18,18	1.46	2 (15%)	16,26,26	2.86	8 (50%)
2	SO4	D	1301	-	4,4,4	0.25	0	6,6,6	0.15	0
3	THM	D	1401	-	13,18,18	1.45	2 (15%)	16,26,26	2.96	9 (56%)
2	SO4	E	1302	-	4,4,4	0.38	0	6,6,6	0.10	0
3	THM	E	1402	-	13,18,18	1.53	3 (23%)	16,26,26	2.96	9 (56%)
2	SO4	F	1304	-	4,4,4	0.13	0	6,6,6	0.07	0
3	THM	F	1404	-	13,18,18	1.52	2 (15%)	16,26,26	2.89	9 (56%)
2	SO4	G	1303	-	4,4,4	0.20	0	6,6,6	0.08	0
3	THM	G	1403	-	13,18,18	1.52	2 (15%)	16,26,26	3.02	9 (56%)
2	SO4	H	1307	-	4,4,4	0.07	0	6,6,6	0.32	0
3	THM	H	1407	-	13,18,18	1.76	4 (30%)	16,26,26	2.93	8 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1300	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1308	-	-	0/0/0/0	0/0/0/0
3	THM	A	1400	-	-	0/2/18/18	0/2/2/2
2	SO4	B	1306	-	-	0/0/0/0	0/0/0/0
3	THM	B	1406	-	-	0/2/18/18	0/2/2/2
2	SO4	C	1305	-	-	0/0/0/0	0/0/0/0
3	THM	C	1405	-	-	0/2/18/18	0/2/2/2
2	SO4	D	1301	-	-	0/0/0/0	0/0/0/0
3	THM	D	1401	-	-	0/2/18/18	0/2/2/2
2	SO4	E	1302	-	-	0/0/0/0	0/0/0/0
3	THM	E	1402	-	-	0/2/18/18	0/2/2/2
2	SO4	F	1304	-	-	0/0/0/0	0/0/0/0
3	THM	F	1404	-	-	0/2/18/18	0/2/2/2
2	SO4	G	1303	-	-	0/0/0/0	0/0/0/0
3	THM	G	1403	-	-	0/2/18/18	0/2/2/2
2	SO4	H	1307	-	-	0/0/0/0	0/0/0/0
3	THM	H	1407	-	-	0/2/18/18	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1402	THM	C5'-C4'	2.05	1.59	1.51
3	H	1407	THM	O3'-C3'	2.16	1.48	1.43
3	H	1407	THM	C5'-C4'	2.26	1.60	1.51
3	A	1400	THM	O4-C4	2.67	1.31	1.24
3	H	1407	THM	O4-C4	2.70	1.31	1.24

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1402	THM	C5-C4-N3	-4.86	119.72	125.14
3	G	1403	THM	C5-C4-N3	-4.80	119.79	125.14
3	C	1405	THM	C5-C4-N3	-4.76	119.83	125.14
3	F	1404	THM	C5-C4-N3	-4.74	119.86	125.14
3	D	1401	THM	C5-C4-N3	-4.72	119.88	125.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1405	THM	1	0
3	D	1401	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%)	0.03	5 (2%) 61 65	20, 37, 59, 97	0
1	B	192/250 (76%)	0.53	24 (12%) 5 5	28, 57, 98, 110	0
1	C	197/250 (78%)	0.49	18 (9%) 11 12	36, 65, 106, 115	0
1	D	191/250 (76%)	0.67	22 (11%) 6 6	41, 72, 103, 114	0
1	E	192/250 (76%)	0.39	10 (5%) 31 35	36, 61, 95, 110	0
1	F	192/250 (76%)	1.00	35 (18%) 2 2	42, 79, 107, 116	0
1	G	192/250 (76%)	0.68	18 (9%) 11 11	32, 69, 108, 123	0
1	H	192/250 (76%)	-0.13	2 (1%) 84 86	21, 35, 55, 71	0
All	All	1545/2000 (77%)	0.46	134 (8%) 13 13	20, 60, 103, 123	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	THR	8.0
1	F	168	ALA	5.7
1	F	95	PRO	5.3
1	F	170	SER	5.2
1	G	206	ASP	5.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	THM	G	1403	17/17	0.94	0.28	1.35	66,70,72,73	0
3	THM	C	1405	17/17	0.92	0.27	0.88	55,58,64,65	0
3	THM	D	1401	17/17	0.96	0.26	0.76	48,51,58,60	0
3	THM	B	1406	17/17	0.96	0.23	0.57	29,37,45,45	0
3	THM	H	1407	17/17	0.98	0.18	0.57	16,26,30,31	0
3	THM	A	1400	17/17	0.97	0.20	0.55	27,31,36,38	0
3	THM	E	1402	17/17	0.96	0.19	-0.04	39,44,52,52	0
3	THM	F	1404	17/17	0.96	0.20	-0.36	45,49,56,58	0
2	SO4	F	1304	5/5	0.96	0.16	-0.73	65,67,68,70	0
2	SO4	H	1307	5/5	0.99	0.14	-0.80	30,31,33,34	0
2	SO4	D	1301	5/5	0.95	0.15	-0.96	55,56,60,61	0
2	SO4	C	1305	5/5	0.98	0.11	-1.02	66,67,68,69	0
2	SO4	B	1306	5/5	0.99	0.12	-1.29	43,44,47,50	0
2	SO4	E	1302	5/5	0.99	0.12	-1.44	49,49,51,52	0
2	SO4	G	1303	5/5	0.97	0.12	-1.97	69,69,69,72	0
2	SO4	A	1300	5/5	0.99	0.09	-2.39	29,29,33,35	0
2	SO4	A	1308	5/5	0.99	0.19	-	43,46,49,50	0

6.5 Other polymers

There are no such residues in this entry.