wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 03:19 PM JST

PDB ID	:	5ZMD
Title	:	Crystal structure of FTO in complex with m6dA modified ssDNA
Authors	:	Zhang, X.; Wei, L.H.; Luo, J.; Xiao, Y.; Liu, J.; Zhang, W.; Zhang, L.; Jia, G.F.
Deposited on	:	2018-04-02
Resolution	:	3.30 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

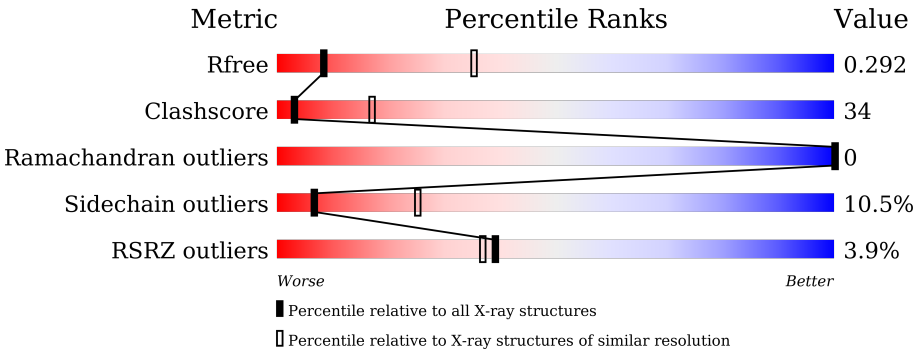
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	463	2% 52% 27% 7% • 13%
1	C	463	5% 38% 37% 10% 15%
1	E	463	4% 45% 35% 5% • 15%
1	G	463	3% 47% 34% 5% • 13%
2	B	9	11% 44% 44%
2	D	9	44% 44% 11%

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Mol	Chain	Length	Quality of chain
2	F	9	33% 44% 22%
2	H	9	44% 44% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OGA	C	1002	-	-	X	-
4	OGA	G	1002	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13828 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 Alpha-ketoglutarate-dependent dioxygenase FTO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3282	2096	569	596	21			
1	C	395	Total	C	N	O	S	0	0	0
			3230	2063	559	588	20			
1	E	395	Total	C	N	O	S	0	0	0
			3228	2063	558	587	20			
1	G	403	Total	C	N	O	S	0	0	0
			3294	2101	573	600	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	LYS	GLN	engineered mutation	UNP Q9C0B1
A	306	LYS	GLN	engineered mutation	UNP Q9C0B1
C	86	LYS	GLN	engineered mutation	UNP Q9C0B1
C	306	LYS	GLN	engineered mutation	UNP Q9C0B1
E	86	LYS	GLN	engineered mutation	UNP Q9C0B1
E	306	LYS	GLN	engineered mutation	UNP Q9C0B1
G	86	LYS	GLN	engineered mutation	UNP Q9C0B1
G	306	LYS	GLN	engineered mutation	UNP Q9C0B1

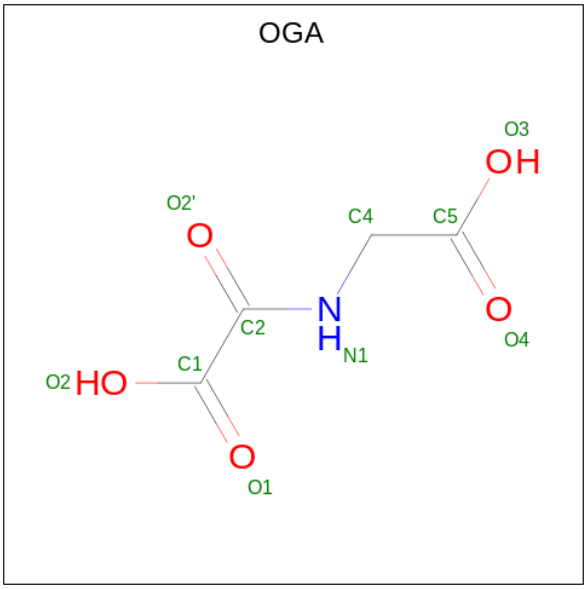
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			183	89	29	56	9			
2	D	9	Total	C	N	O	P	0	0	0
			183	89	29	56	9			
2	F	9	Total	C	N	O	P	0	0	0
			183	89	29	56	9			
2	H	9	Total	C	N	O	P	0	0	0
			183	89	29	56	9			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	G	1	Total Mn 1 1	0	0

- Molecule 4 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 10 4 1 5	0	0
4	C	1	Total C N O 10 4 1 5	0	0
4	E	1	Total C N O 10 4 1 5	0	0
4	G	1	Total C N O 10 4 1 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0

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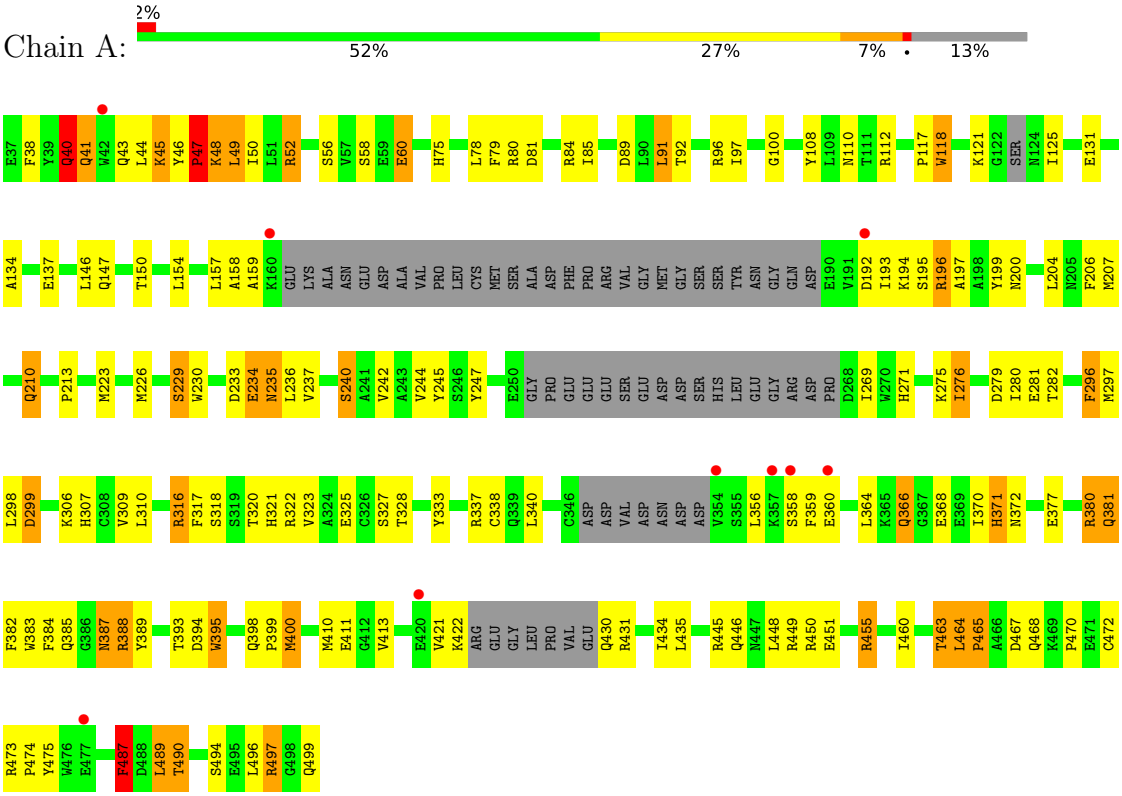
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	3	Total O 3 3	0	0
5	D	2	Total O 2 2	0	0
5	E	1	Total O 1 1	0	0
5	G	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

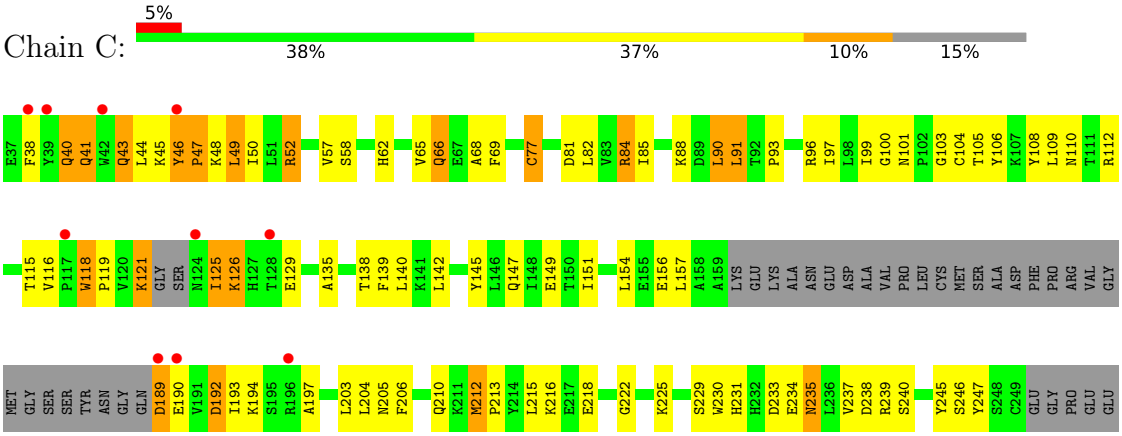
• Molecule 1: Alpha-ketoglutarate-dependent dioxygenase FTO

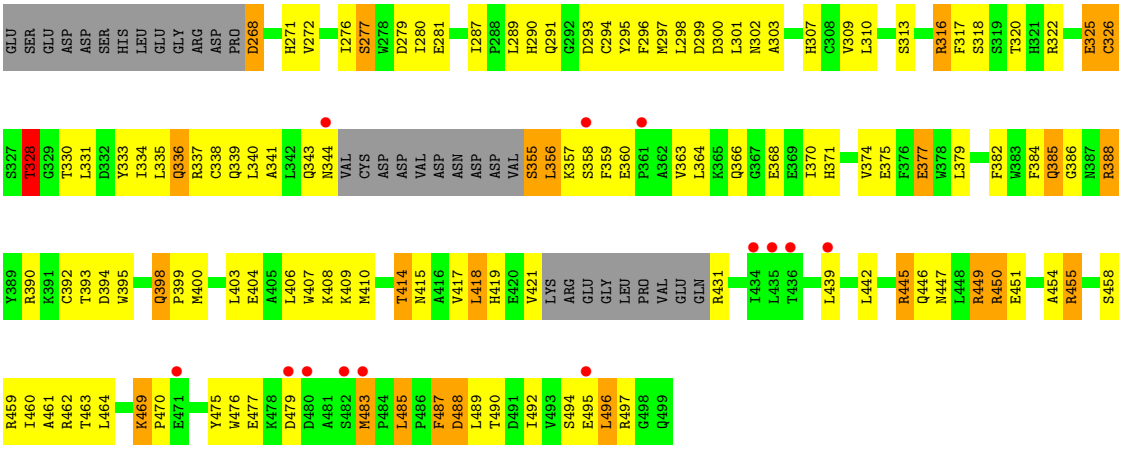
Chain A:



• Molecule 1: Alpha-ketoglutarate-dependent dioxygenase FTO

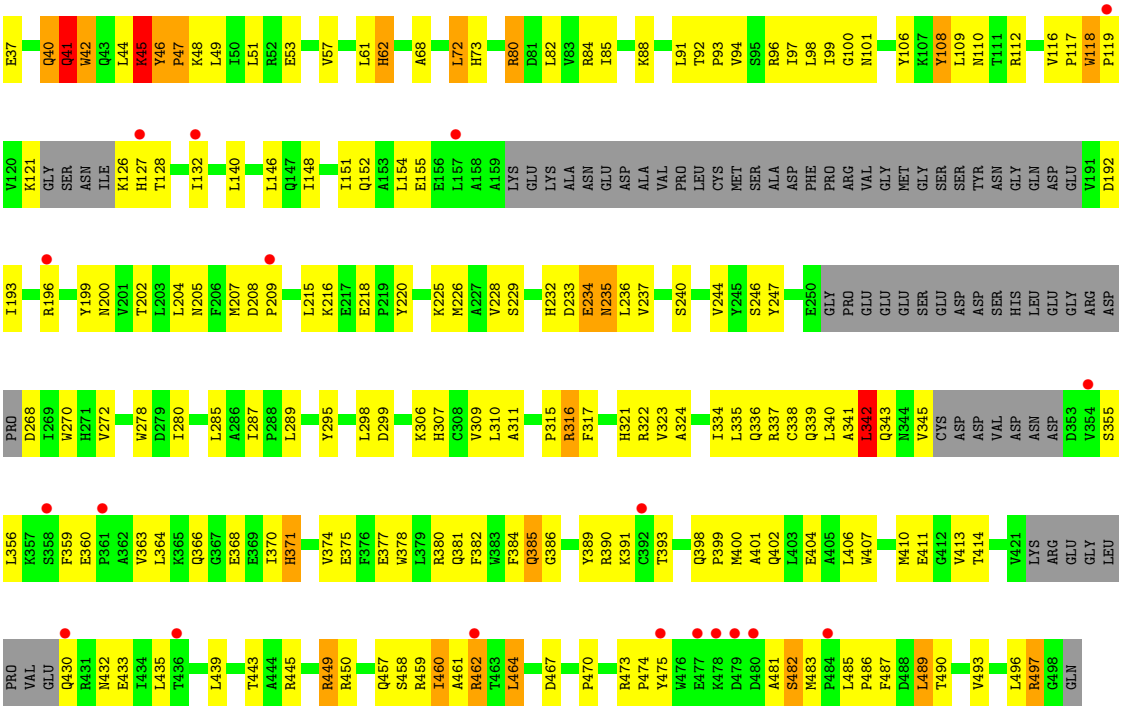
Chain C:





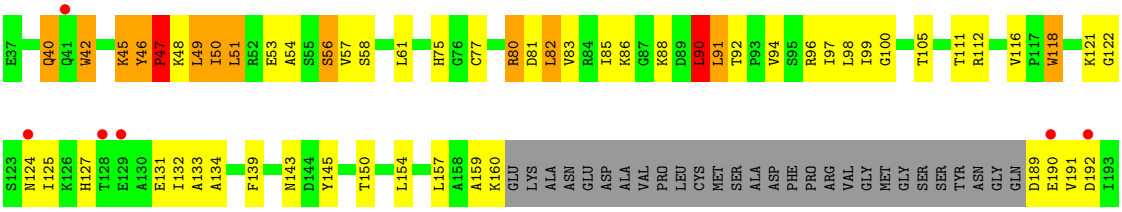
• Molecule 1: Alpha-ketoglutarate-dependent dioxygenase FTO

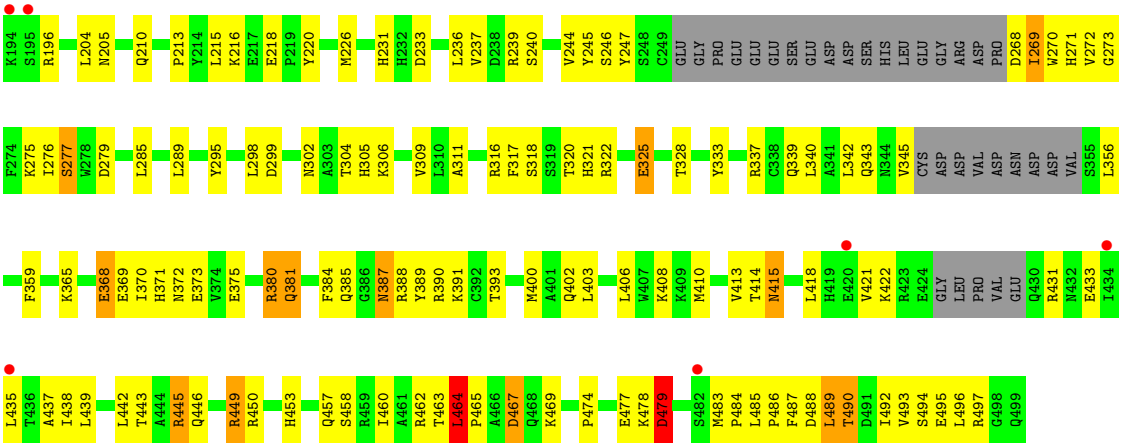
Chain E:



• Molecule 1: Alpha-ketoglutarate-dependent dioxygenase FTO

Chain G:



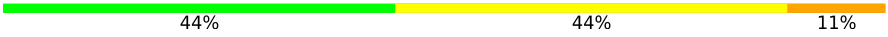


• Molecule 2: DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3')

Chain B:

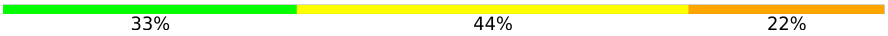
• Molecule 2: DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3')

Chain D:



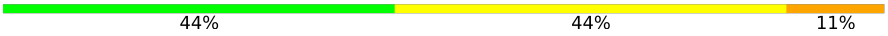
• Molecule 2: DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3')

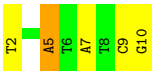
Chain F:



• Molecule 2: DNA (5'-D(P*TP*CP*TP*(6MA)P*TP*AP*TP*CP*G)-3')

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.74Å 160.03Å 276.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.17 – 3.30 36.90 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.17-3.30) 99.4 (36.90-3.30)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.271 , 0.292 0.273 , 0.292	Depositor DCC
R_{free} test set	2060 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	75.6	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 26.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13828	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4472e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OGA, 6MA, MN

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	0.88	3/3361 (0.1%)	0.95	11/4550 (0.2%)
1	C	0.88	5/3309 (0.2%)	0.93	9/4482 (0.2%)
1	E	0.63	0/3307	0.86	13/4480 (0.3%)
1	G	0.73	2/3374 (0.1%)	0.95	17/4568 (0.4%)
2	B	1.60	3/177 (1.7%)	1.31	2/268 (0.7%)
2	D	0.61	0/177	1.11	0/268
2	F	0.77	1/177 (0.6%)	1.14	0/268
2	H	0.61	0/177	1.15	0/268
All	All	0.80	14/14059 (0.1%)	0.94	52/19152 (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	E	0	1
1	G	0	1
All	All	0	2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	DT	O3'-P	-13.23	1.45	1.61
1	C	395	TRP	CB-CG	-9.39	1.33	1.50
1	C	43	GLN	C-N	8.17	1.52	1.34
1	A	234	GLU	CD-OE1	-6.56	1.18	1.25
1	C	395	TRP	CD2-CE2	-6.08	1.34	1.41

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	PRO	N-CA-C	13.17	146.33	112.10
1	A	47	PRO	CB-CA-C	-10.81	84.98	112.00
1	G	46	TYR	C-N-CD	-9.90	98.83	120.60
1	E	46	TYR	N-CA-C	9.62	136.97	111.00
1	C	485	LEU	C-N-CD	-9.55	99.59	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	45	LYS	Mainchain
1	G	45	LYS	Mainchain

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	3282	0	3226	184	1
1	C	3230	0	3164	287	0
1	E	3228	0	3161	212	0
1	G	3294	0	3237	229	1
2	B	183	0	106	8	0
2	D	183	0	106	7	0
2	F	183	0	106	11	0
2	H	183	0	106	10	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	10	0	3	3	0
4	C	10	0	3	4	0
4	E	10	0	3	0	0
4	G	10	0	3	5	0
5	A	10	0	0	1	0
5	C	3	0	0	1	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13828	0	13224	912	1

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 34.

The worst 5 of 912 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:46:TYR:HB3	1:G:47:PRO:CD	1.24	1.56
1:C:46:TYR:CB	1:C:47:PRO:HD3	1.15	1.45
1:G:46:TYR:CB	1:G:47:PRO:HD3	1.27	1.43
1:E:46:TYR:HB3	1:E:47:PRO:CD	1.04	1.41
1:E:46:TYR:CB	1:E:47:PRO:HD3	1.16	1.39

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:O	1:G:58:SER:OG[7_555]	2.01	0.19

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	390/463 (84%)	353 (90%)	37 (10%)	0	100	100
1	C	383/463 (83%)	356 (93%)	27 (7%)	0	100	100
1	E	383/463 (83%)	349 (91%)	34 (9%)	0	100	100
1	G	393/463 (85%)	355 (90%)	38 (10%)	0	100	100
All	All	1549/1852 (84%)	1413 (91%)	136 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	356/408 (87%)	317 (89%)	39 (11%)	6 24
1	C	350/408 (86%)	297 (85%)	53 (15%)	3 13
1	E	350/408 (86%)	323 (92%)	27 (8%)	13 38
1	G	357/408 (88%)	328 (92%)	29 (8%)	11 36
All	All	1413/1632 (87%)	1265 (90%)	148 (10%)	7 25

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	467	ASP
1	G	464	LEU
1	G	40	GLN
1	G	118	TRP
1	C	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	302	ASN
1	G	381	GLN
1	G	453	HIS
1	G	446	GLN
1	C	339	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	6MA	B	5	2	18,24,25	0.92	1 (5%)	15,34,37	2.11	4 (26%)
2	6MA	D	5	2	18,24,25	0.93	1 (5%)	15,34,37	2.17	4 (26%)
2	6MA	F	5	2	18,24,25	0.94	1 (5%)	15,34,37	2.08	4 (26%)
2	6MA	H	5	2	18,24,25	0.90	1 (5%)	15,34,37	2.16	4 (26%)

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	6MA	B	5	2	-	0/5/23/24	0/3/3/3
2	6MA	D	5	2	-	0/5/23/24	0/3/3/3
2	6MA	F	5	2	-	0/5/23/24	0/3/3/3
2	6MA	H	5	2	-	0/5/23/24	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	6MA	C5-C4	2.52	1.47	1.40
2	D	5	6MA	C5-C4	2.48	1.47	1.40
2	B	5	6MA	C5-C4	2.45	1.47	1.40
2	H	5	6MA	C5-C4	2.42	1.47	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	6MA	C2-N1-C6	5.98	121.72	116.59
2	F	5	6MA	C2-N1-C6	5.94	121.68	116.59
2	B	5	6MA	C2-N1-C6	5.92	121.67	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5	6MA	C2-N1-C6	5.88	121.63	116.59
2	D	5	6MA	C1-N6-C6	-3.60	119.77	122.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5	6MA	1	0
2	D	5	6MA	2	0
2	F	5	6MA	3	0
2	H	5	6MA	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	OGA	C	1002	3	9,9,9	4.51	3 (33%)	10,11,11	2.24	1 (10%)
4	OGA	E	1002	3	9,9,9	4.48	3 (33%)	10,11,11	2.23	2 (20%)
4	OGA	A	1002	3	9,9,9	4.50	3 (33%)	10,11,11	2.48	3 (30%)
4	OGA	G	1002	3	9,9,9	4.50	3 (33%)	10,11,11	2.47	4 (40%)

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
4	OGA	C	1002	3	-	0/8/9/9	-
4	OGA	E	1002	3	-	0/8/9/9	-
4	OGA	A	1002	3	-	0/8/9/9	-
4	OGA	G	1002	3	-	0/8/9/9	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	OGA	C2-N1	11.17	1.52	1.33
4	C	1002	OGA	C2-N1	11.16	1.52	1.33
4	G	1002	OGA	C2-N1	11.15	1.52	1.33
4	E	1002	OGA	C2-N1	11.09	1.52	1.33
4	G	1002	OGA	C2-C1	-6.47	1.46	1.54

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1002	OGA	C4-N1-C2	-6.25	111.47	121.25
4	A	1002	OGA	C4-N1-C2	-6.25	111.47	121.25
4	E	1002	OGA	C4-N1-C2	-6.24	111.49	121.25
4	G	1002	OGA	C4-N1-C2	-6.21	111.52	121.25
4	A	1002	OGA	O2-C1-C2	2.37	120.14	113.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1002	OGA	4	0
4	A	1002	OGA	3	0
4	G	1002	OGA	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	402/463 (86%)	0.15	9 (2%) 62 60	13, 27, 52, 64	0
1	C	395/463 (85%)	0.27	23 (5%) 23 22	14, 31, 57, 70	0
1	E	395/463 (85%)	0.34	19 (4%) 30 28	17, 34, 54, 80	0
1	G	403/463 (87%)	0.15	12 (2%) 50 49	11, 26, 52, 75	0
2	B	8/9 (88%)	-0.03	0 100 100	13, 22, 29, 43	0
2	D	8/9 (88%)	0.05	0 100 100	13, 24, 31, 51	0
2	F	8/9 (88%)	0.06	0 100 100	13, 24, 27, 45	0
2	H	8/9 (88%)	0.06	0 100 100	13, 18, 30, 45	0
All	All	1627/1888 (86%)	0.22	63 (3%) 39 37	11, 29, 54, 80	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	VAL	4.9
1	C	434	ILE	4.7
1	G	128	THR	4.6
1	G	124	ASN	4.6
1	C	128	THR	4.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6MA	D	5	22/23	0.95	0.21	8,16,24,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6MA	F	5	22/23	0.95	0.23	6,21,33,40	0
2	6MA	B	5	22/23	0.96	0.28	8,14,21,23	0
2	6MA	H	5	22/23	0.96	0.23	5,12,15,17	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	G	1001	1/1	0.80	0.34	13,13,13,13	0
4	OGA	G	1002	10/10	0.84	0.37	10,12,20,30	0
4	OGA	C	1002	10/10	0.88	0.38	12,18,26,29	0
3	MN	C	1001	1/1	0.88	0.16	17,17,17,17	0
3	MN	E	1001	1/1	0.93	0.21	20,20,20,20	0
3	MN	A	1001	1/1	0.94	0.24	12,12,12,12	0
4	OGA	A	1002	10/10	0.95	0.29	8,16,21,32	0
4	OGA	E	1002	10/10	0.96	0.27	14,22,24,29	0

6.5 Other polymers (i)

There are no such residues in this entry.