wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 04:26 AM EDT

PDB ID	:	6HC3
Title	:	TFAM bound to Site-X
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Deposited on	:	2018-08-13
Resolution	:	3.10 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 (i)) were used in the production of this report:

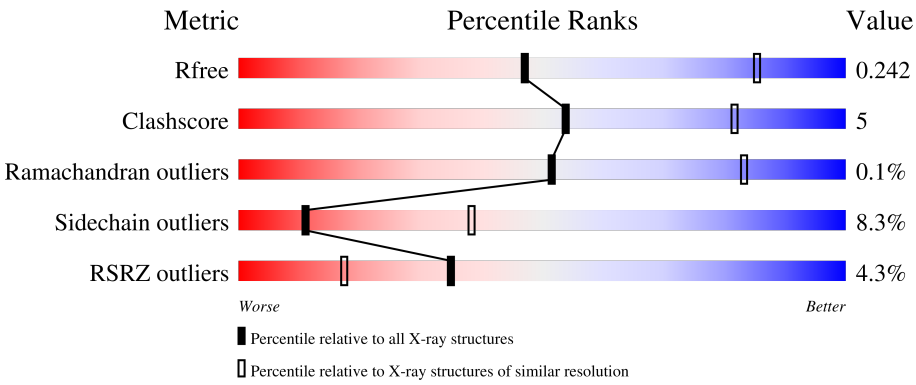
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	224	71% 14% • 14%
1	D	224	9% 63% 20% • 14%
1	G	224	9% 70% 15% 14%
1	J	224	72% 12% 15%
2	B	22	27% 59% 14%

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Mol	Chain	Length	Quality of chain
2	E	22	18% 73% 9%
2	H	22	18% 59% 23%
2	K	22	36% 55% 9%
3	C	22	45% 50% 5%
3	F	22	36% 59% 5%
3	I	22	36% 50% 14%
3	L	22	36% 55% 9%

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	TLA	A	303	-	-	-	X
5	1PE	J	301	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10557 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 Transcription factor A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	192	1610	1016	291	297	6	0	0	0
1	D	192	1747	1102	312	327	6	0	15	0
1	G	192	1729	1091	309	323	6	0	13	0
1	J	191	1609	1016	290	297	6	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP Q00059
A	32	GLY	-	cloning artifact	UNP Q00059
A	33	SER	-	cloning artifact	UNP Q00059
A	247	LEU	-	cloning artifact	UNP Q00059
A	248	GLN	-	cloning artifact	UNP Q00059
A	249	HIS	-	expression tag	UNP Q00059
A	250	HIS	-	expression tag	UNP Q00059
A	251	HIS	-	expression tag	UNP Q00059
A	252	HIS	-	expression tag	UNP Q00059
A	253	HIS	-	expression tag	UNP Q00059
A	254	HIS	-	expression tag	UNP Q00059
D	31	MET	-	initiating methionine	UNP Q00059
D	32	GLY	-	cloning artifact	UNP Q00059
D	33	SER	-	cloning artifact	UNP Q00059
D	247	LEU	-	cloning artifact	UNP Q00059
D	248	GLN	-	cloning artifact	UNP Q00059
D	249	HIS	-	expression tag	UNP Q00059
D	250	HIS	-	expression tag	UNP Q00059
D	251	HIS	-	expression tag	UNP Q00059
D	252	HIS	-	expression tag	UNP Q00059
D	253	HIS	-	expression tag	UNP Q00059

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Chain	Residue	Modelled	Actual	Comment	Reference
D	254	HIS	-	expression tag	UNP Q00059
G	31	MET	-	initiating methionine	UNP Q00059
G	32	GLY	-	cloning artifact	UNP Q00059
G	33	SER	-	cloning artifact	UNP Q00059
G	247	LEU	-	cloning artifact	UNP Q00059
G	248	GLN	-	cloning artifact	UNP Q00059
G	249	HIS	-	expression tag	UNP Q00059
G	250	HIS	-	expression tag	UNP Q00059
G	251	HIS	-	expression tag	UNP Q00059
G	252	HIS	-	expression tag	UNP Q00059
G	253	HIS	-	expression tag	UNP Q00059
G	254	HIS	-	expression tag	UNP Q00059
J	31	MET	-	initiating methionine	UNP Q00059
J	32	GLY	-	cloning artifact	UNP Q00059
J	33	SER	-	cloning artifact	UNP Q00059
J	247	LEU	-	cloning artifact	UNP Q00059
J	248	GLN	-	cloning artifact	UNP Q00059
J	249	HIS	-	expression tag	UNP Q00059
J	250	HIS	-	expression tag	UNP Q00059
J	251	HIS	-	expression tag	UNP Q00059
J	252	HIS	-	expression tag	UNP Q00059
J	253	HIS	-	expression tag	UNP Q00059
J	254	HIS	-	expression tag	UNP Q00059

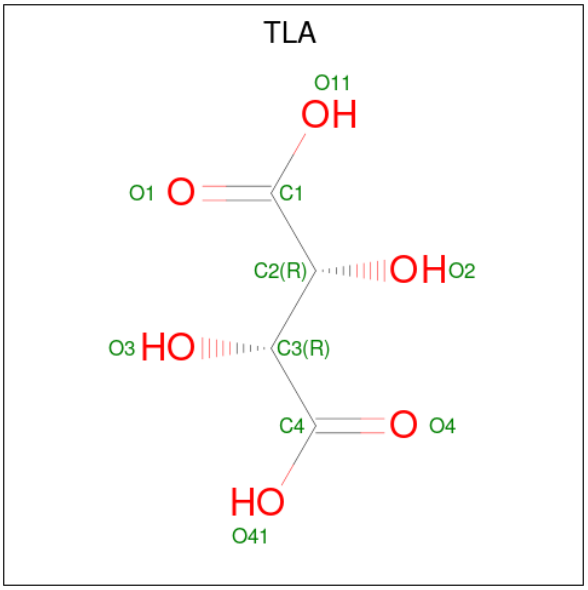
- Molecule 2 is a DNA chain called DNA/RNA (5'-D(*TP*AP*AP*CP*AP*AP*AP*AP*AP*AP*AP*TP*TP*TP*CP*CP*AP*CP*CP*AP*AP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	22	443	214	86	122	21	0	0	0
			Total	C	N	O	P			
2	E	22	443	214	86	122	21	0	0	0
			Total	C	N	O	P			
2	H	22	602	290	115	168	29	0	8	0
			Total	C	N	O	P			
2	K	22	443	214	86	122	21	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*TP*TP*GP*GP*TP*GP*GP*AP*AP*AP*TP*TP*TP*TP*TP*TP*GP*TP*TP*AP*G)-3').

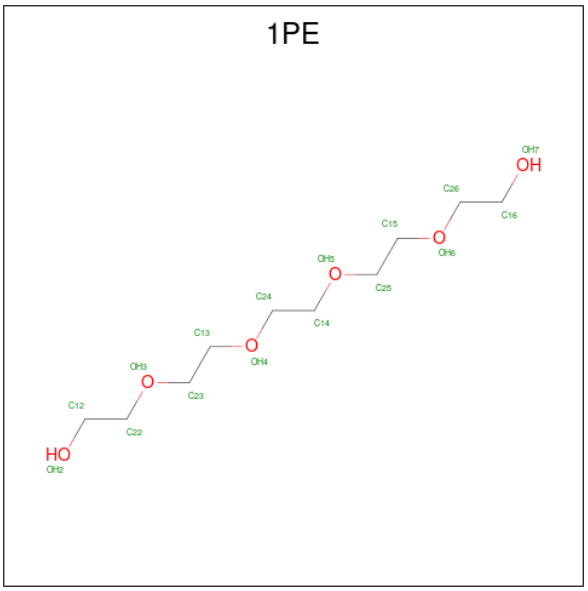
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	22	453	220	74	138	21	0	0	0
3	F	22	453	220	74	138	21	0	0	0
3	I	22	453	220	74	138	21	0	0	0
3	L	22	453	220	74	138	21	0	0	0

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	4	6	0	0
4	A	1	10	4	6	0	0
4	A	1	10	4	6	0	0
4	D	1	10	4	6	0	0
4	G	1	10	4	6	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	12	8	4	0	0
			Total	C	O		
5	D	1	15	10	5	0	0
			Total	C	O		
5	G	1	15	10	5	0	0
			Total	C	O		
5	J	1	15	10	5	0	0

- Molecule 6 is water.

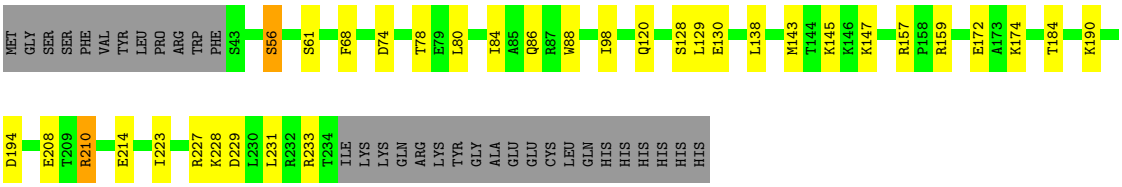
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	3	3	3	0	0
			Total	O		
6	B	1	1	1	0	0
			Total	O		
6	C	1	1	1	0	0
			Total	O		
6	D	1	1	1	0	0
			Total	O		
6	F	1	1	1	0	0
			Total	O		
6	G	2	2	2	0	0
			Total	O		
6	J	3	3	3	0	0

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.

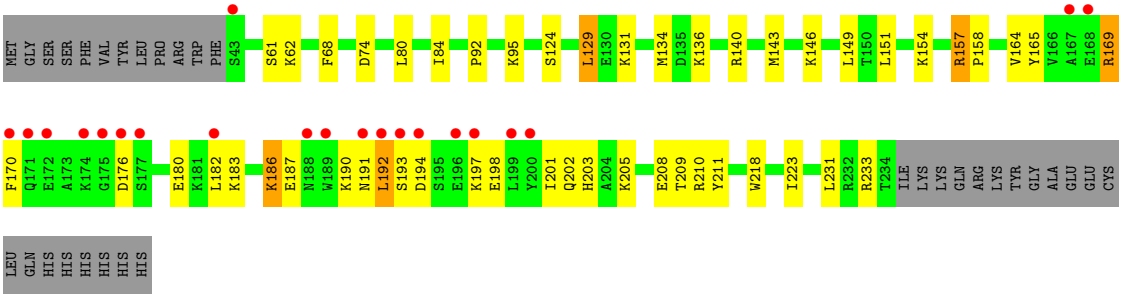
• Molecule 1: Transcription factor A, mitochondrial

Chain A:



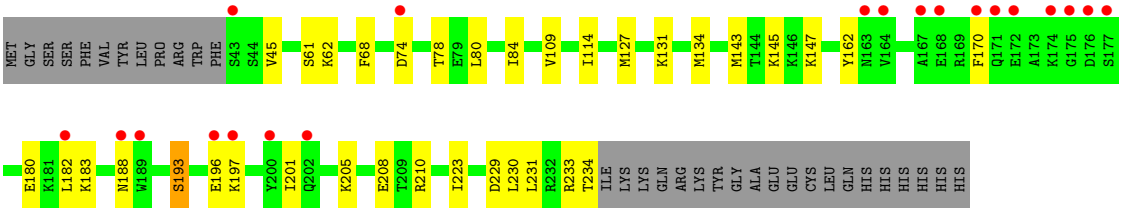
• Molecule 1: Transcription factor A, mitochondrial

Chain D:



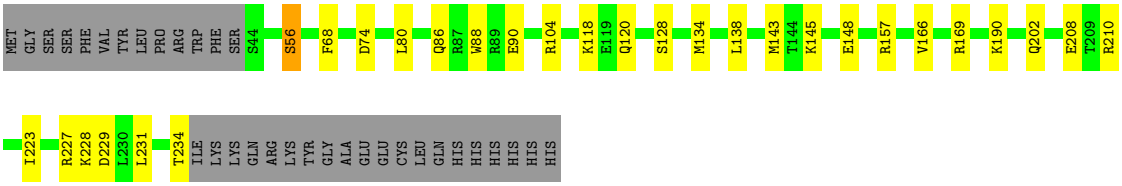
• Molecule 1: Transcription factor A, mitochondrial

Chain G:



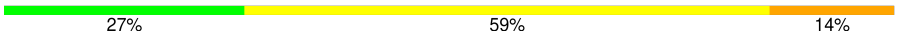
• Molecule 1: Transcription factor A, mitochondrial

Chain J:



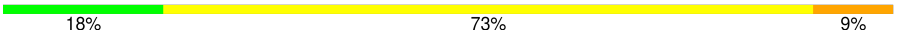
• Molecule 2: DNA/RNA (5'-D(*TP*AP*AP*CP*AP*AP*AP*AP*AP*AP*TP*TP*TP*CP*CP*AP*CP*CP*AP*AP*AP*C)-3')

Chain B:



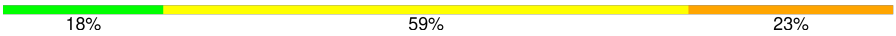
• Molecule 2: DNA/RNA (5'-D(*TP*AP*AP*CP*AP*AP*AP*AP*AP*AP*TP*TP*TP*CP*CP*AP*CP*CP*AP*AP*AP*C)-3')

Chain E:



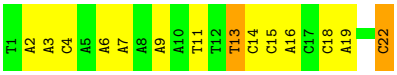
• Molecule 2: DNA/RNA (5'-D(*TP*AP*AP*CP*AP*AP*AP*AP*AP*AP*TP*TP*TP*CP*CP*AP*CP*CP*AP*AP*AP*C)-3')

Chain H:



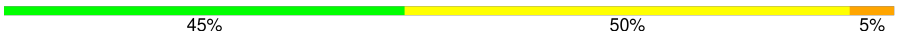
• Molecule 2: DNA/RNA (5'-D(*TP*AP*AP*CP*AP*AP*AP*AP*AP*AP*TP*TP*TP*CP*CP*AP*CP*CP*AP*AP*AP*C)-3')

Chain K:



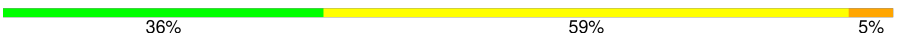
• Molecule 3: DNA (5'-D(*TP*TP*TP*GP*GP*TP*GP*GP*AP*AP*AP*TP*TP*TP*TP*TP*TP*GP*TP*TP*AP*G)-3')

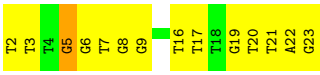
Chain C:



• Molecule 3: DNA (5'-D(*TP*TP*TP*GP*GP*TP*GP*GP*AP*AP*AP*TP*TP*TP*TP*TP*TP*GP*TP*TP*AP*G)-3')

Chain F:





• Molecule 3: DNA (5'-D(*TP*TP*TP*GP*GP*TP*GP*GP*AP*AP*AP*TP*TP*TP*TP*TP*TP*GP*TP*TP*AP*G)-3')

Chain I:

• Molecule 3: DNA (5'-D(*TP*TP*TP*GP*GP*TP*GP*GP*AP*AP*AP*TP*TP*TP*TP*TP*TP*GP*TP*TP*AP*G)-3')

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.79Å 145.14Å 108.12Å 90.00° 130.83° 90.00°	Depositor
Resolution (Å)	42.21 – 3.10 40.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.21-3.10) 98.0 (40.78-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.188 , 0.229 0.198 , 0.242	Depositor DCC
R_{free} test set	1732 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 26.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.468 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10557	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, TLA

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	0.60	0/1641	0.69	0/2196
1	D	0.67	0/1781	0.74	0/2383
1	G	0.63	0/1763	0.68	0/2360
1	J	0.60	0/1640	0.72	1/2194 (0.0%)
2	B	1.37	2/498 (0.4%)	2.07	23/764 (3.0%)
2	E	1.34	2/498 (0.4%)	2.08	33/764 (4.3%)
2	H	1.19	0/676	2.13	40/1037 (3.9%)
2	K	1.38	1/498 (0.2%)	2.04	21/764 (2.7%)
3	C	1.23	1/506 (0.2%)	2.16	24/782 (3.1%)
3	F	1.23	3/506 (0.6%)	2.06	25/782 (3.2%)
3	I	1.18	0/506	1.97	20/782 (2.6%)
3	L	1.24	3/506 (0.6%)	2.16	26/782 (3.3%)
All	All	0.93	12/11019 (0.1%)	1.45	213/15590 (1.4%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	19	DA	C3'-O3'	-6.21	1.35	1.44
3	L	22	DA	C3'-O3'	-6.05	1.36	1.44
2	E	20	DA	C3'-O3'	-5.64	1.36	1.44
3	C	22	DA	C3'-O3'	-5.58	1.36	1.44
2	K	4	DC	C3'-O3'	-5.23	1.37	1.44

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	15[A]	DC	O4'-C1'-N1	11.82	116.27	108.00
2	H	15[B]	DC	O4'-C1'-N1	11.82	116.27	108.00
3	L	7	DT	C4-C5-C7	10.76	125.46	119.00
3	C	2	DT	O4'-C1'-N1	9.62	114.73	108.00
2	H	14[A]	DC	O4'-C1'-N1	9.49	114.65	108.00

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	1610	0	1646	13	0
1	D	1747	0	1776	45	0
1	G	1729	0	1759	18	0
1	J	1609	0	1650	18	1
2	B	443	0	248	4	0
2	E	443	0	248	3	0
2	H	602	0	337	12	0
2	K	443	0	248	2	0
3	C	453	0	256	1	0
3	F	453	0	256	2	0
3	I	453	0	256	6	0
3	L	453	0	256	4	0
4	A	30	0	12	0	0
4	D	10	0	4	0	0
4	G	10	0	4	0	0
5	A	12	0	15	1	0
5	D	15	0	19	3	0
5	G	15	0	19	0	0
5	J	15	0	19	9	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	J	3	0	0	0	0
All	All	10557	0	9028	103	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 5.

The worst 5 of 103 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:183:LYS:O	1:D:186[B]:LYS:HE3	1.27	1.33
1:D:183:LYS:O	1:D:186[B]:LYS:CE	1.99	1.10
1:D:183:LYS:HA	1:D:186[B]:LYS:HE2	1.43	0.99
1:D:186[B]:LYS:HD3	1:D:187[B]:GLU:H	1.25	0.98
1:D:186[B]:LYS:HD3	1:D:187[B]:GLU:N	1.83	0.92

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:J:86:GLN:NE2	1:J:90:GLU:OE1[2_656]	2.15	0.05

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	190/224 (85%)	187 (98%)	3 (2%)	0	100	100
1	D	205/224 (92%)	195 (95%)	10 (5%)	0	100	100
1	G	203/224 (91%)	195 (96%)	6 (3%)	2 (1%)	15	49
1	J	189/224 (84%)	185 (98%)	4 (2%)	0	100	100
All	All	787/896 (88%)	762 (97%)	23 (3%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	188[A]	ASN
1	G	188[B]	ASN

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	176/207 (85%)	159 (90%)	17 (10%)	8	30
1	D	193/207 (93%)	170 (88%)	23 (12%)	5	20
1	G	191/207 (92%)	178 (93%)	13 (7%)	16	45
1	J	177/207 (86%)	164 (93%)	13 (7%)	14	43
All	All	737/828 (89%)	671 (91%)	66 (9%)	11	34

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	143	MET
1	J	169	ARG
1	J	234	THR
1	D	169	ARG
1	D	157	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
4	TLA	A	303	-	9,9,9	1.39	2 (22%)	12,12,12	1.23	2 (16%)
5	1PE	G	302	-	14,14,15	0.69	0	13,13,14	0.65	0
4	TLA	A	302	-	9,9,9	1.95	4 (44%)	12,12,12	1.77	4 (33%)
5	1PE	J	301	-	14,14,15	0.81	0	13,13,14	0.68	0
5	1PE	A	304	-	11,11,15	0.65	0	10,10,14	0.85	0
4	TLA	D	301	-	9,9,9	1.98	4 (44%)	12,12,12	1.83	4 (33%)
5	1PE	D	302	-	14,14,15	0.75	0	13,13,14	0.70	0
4	TLA	A	301	-	9,9,9	1.95	4 (44%)	12,12,12	1.73	4 (33%)
4	TLA	G	301	-	9,9,9	1.42	2 (22%)	12,12,12	1.45	2 (16%)

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	TLA	A	303	-	-	0/12/12/12	-
5	1PE	G	302	-	-	2/12/12/13	-
4	TLA	A	302	-	-	0/12/12/12	-
5	1PE	J	301	-	-	5/12/12/13	-
5	1PE	A	304	-	-	1/9/9/13	-
4	TLA	D	301	-	-	0/12/12/12	-
5	1PE	D	302	-	-	2/12/12/13	-
4	TLA	A	301	-	-	0/12/12/12	-
4	TLA	G	301	-	-	1/12/12/12	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	TLA	O1-C1	3.77	1.33	1.22
4	A	302	TLA	O4-C4	3.42	1.32	1.22
4	G	301	TLA	O4-C4	3.41	1.32	1.22
4	A	303	TLA	O1-C1	3.31	1.31	1.22
4	A	301	TLA	O4-C4	3.19	1.31	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	301	TLA	O41-C4-C3	3.36	122.63	113.31
4	G	301	TLA	O41-C4-C3	3.25	122.33	113.31
4	A	302	TLA	O11-C1-C2	3.23	122.28	113.31
4	D	301	TLA	O11-C1-C2	3.15	122.06	113.31
4	A	301	TLA	O11-C1-C2	3.13	122.00	113.31

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	302	1PE	C25-C15-OH6-C26
5	J	301	1PE	C13-C23-OH3-C22
5	J	301	1PE	C23-C13-OH4-C24
5	J	301	1PE	C25-C15-OH6-C26
5	G	302	1PE	OH2-C12-C22-OH3

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	301	1PE	9	0
5	A	304	1PE	1	0
5	D	302	1PE	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	192/224 (85%)	-0.26	0 100 100	20, 49, 103, 134	0
1	D	192/224 (85%)	0.21	21 (10%) 5 2	15, 44, 156, 176	3 (1%)
1	G	192/224 (85%)	0.26	20 (10%) 6 2	15, 46, 135, 167	0
1	J	191/224 (85%)	-0.28	0 100 100	17, 49, 106, 130	0
2	B	22/22 (100%)	-0.52	0 100 100	40, 48, 66, 71	0
2	E	22/22 (100%)	-0.44	0 100 100	36, 72, 118, 127	0
2	H	22/22 (100%)	-0.27	0 100 100	37, 64, 84, 87	0
2	K	22/22 (100%)	-0.60	0 100 100	40, 48, 66, 73	0
3	C	22/22 (100%)	-0.52	0 100 100	33, 46, 65, 73	0
3	F	22/22 (100%)	-0.33	0 100 100	19, 76, 109, 113	0
3	I	22/22 (100%)	-0.35	0 100 100	20, 76, 112, 114	0
3	L	22/22 (100%)	-0.55	0 100 100	35, 45, 67, 77	0
All	All	943/1072 (87%)	-0.10	41 (4%) 35 17	15, 49, 127, 176	3 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	176	ASP	7.3
1	G	177	SER	5.8
1	D	200[A]	TYR	5.2
1	D	189[A]	TRP	5.0
1	G	174	LYS	4.8

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	TLA	A	303	10/10	0.65	0.52	125,132,135,137	0
4	TLA	A	302	10/10	0.71	0.35	143,145,147,147	0
4	TLA	A	301	10/10	0.71	0.34	133,136,139,139	0
4	TLA	D	301	10/10	0.79	0.30	82,89,92,94	0
5	1PE	J	301	15/16	0.85	0.41	71,74,77,78	0
5	1PE	D	302	15/16	0.86	0.33	52,61,66,67	0
5	1PE	A	304	12/16	0.87	0.32	71,73,80,81	0
5	1PE	G	302	15/16	0.89	0.40	50,56,58,59	0
4	TLA	G	301	10/10	0.90	0.13	72,79,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.