Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:47 AM BST

PDB ID	:	4DNC
Title	:	Crystal structure of human MOF in complex with MSL1
Authors	:	Huang, J.; Lei, M.
Deposited on	:	2012-02-08
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

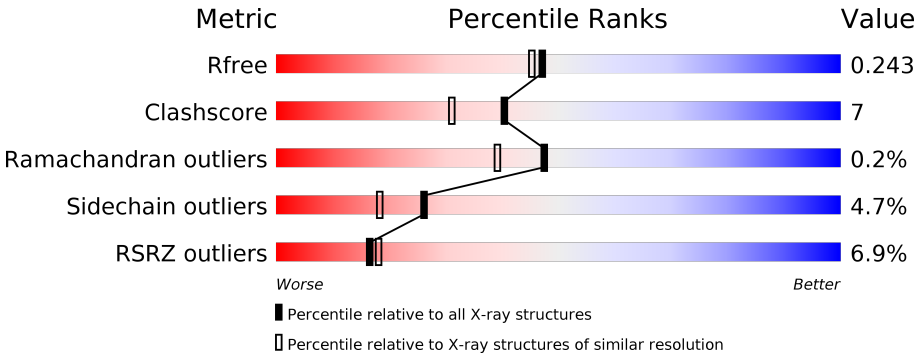
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	289	5% 80% 12% • 6%
1	B	289	4% 79% 13% • 7%
2	D	48	13% 63% 23% • 13%
2	E	48	23% 67% 29% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5372 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 Histone acetyltransferase KAT8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	1	0	0
			2256	1476	366	403	11			
1	B	268	Total	C	N	O	S	0	0	0
			2223	1452	360	400	11			

- Molecule 2 is a protein called Male-specific lethal 1 homolog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	42	Total	C	N	O	0	0	0
			352	217	70	65			
2	E	46	Total	C	N	O	0	0	0
			388	243	73	72			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

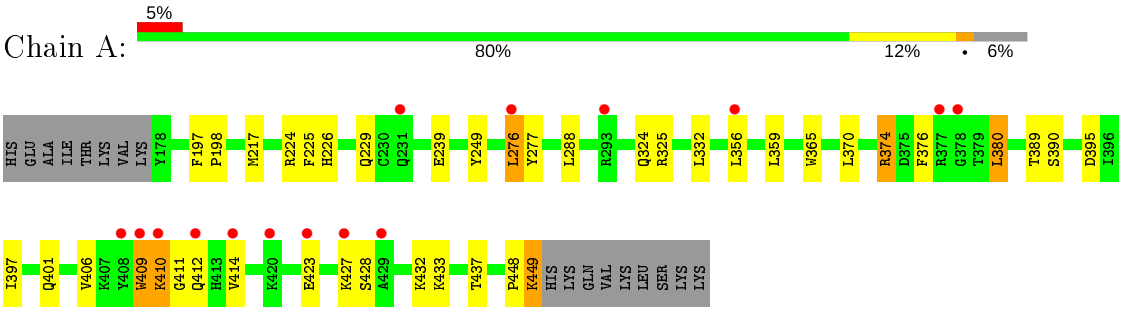
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	62	Total	O	0	0
			62	62		
4	D	5	Total	O	0	0
			5	5		
4	E	10	Total	O	0	0
			10	10		

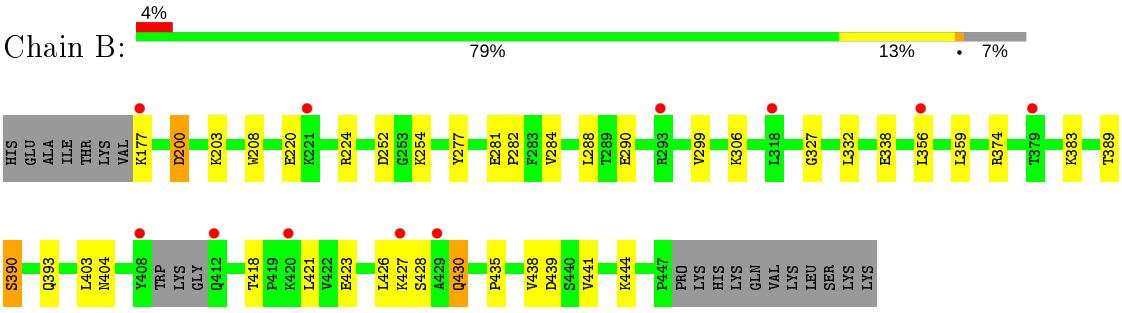
3 Residue-property plots (i)

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.

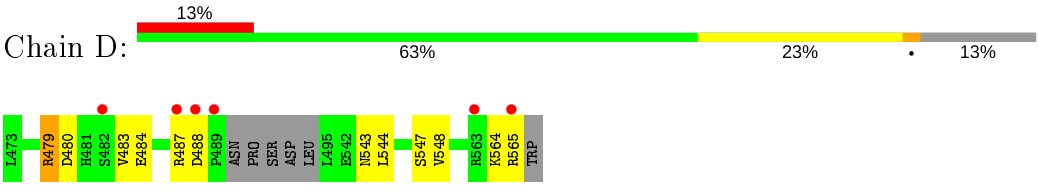
- Molecule 1: Histone acetyltransferase KAT8



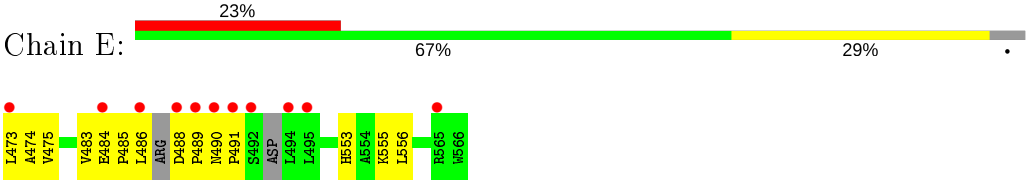
- Molecule 1: Histone acetyltransferase KAT8



- Molecule 2: Male-specific lethal 1 homolog



- Molecule 2: Male-specific lethal 1 homolog



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.80Å 111.52Å 66.75Å 90.00° 111.05° 90.00°	Depositor
Resolution (Å)	40.99 – 2.05 40.99 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.9 (40.99-2.05) 97.9 (40.99-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.208 , 0.246 0.208 , 0.243	Depositor DCC
R_{free} test set	5530 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5372	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ALY

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	0.41	0/2311	0.53	0/3131
1	B	0.42	0/2274	0.55	0/3078
2	D	0.30	0/358	0.44	0/479
2	E	0.36	0/396	0.47	0/531
All	All	0.40	0/5339	0.53	0/7219

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

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	2256	0	2242	30	0
1	B	2223	0	2207	26	0
2	D	352	0	346	9	0
2	E	388	0	380	22	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	74	0	0	0	0
4	B	62	0	0	0	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	10	0	0	0	0
All	All	5372	0	5175	75	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 7.

All (75) 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)
2:E:473:LEU:HG	2:E:474:ALA:H	1.27	1.00
2:E:473:LEU:HG	2:E:474:ALA:N	1.87	0.87
2:E:485:PRO:O	2:E:486:LEU:HB2	1.77	0.85
1:A:448:PRO:O	1:A:449:LYS:HB2	1.84	0.76
1:B:177:LYS:N	1:B:203:LYS:HZ1	1.84	0.76
1:A:239:GLU:HB2	1:A:249:TYR:CE1	2.22	0.74
2:E:473:LEU:CG	2:E:474:ALA:H	2.00	0.73
2:D:479:ARG:HH11	2:D:479:ARG:HB3	1.57	0.69
1:B:284:VAL:HG23	1:B:306:LYS:HG3	1.74	0.68
2:E:489:PRO:HB2	2:E:491:PRO:HD3	1.74	0.68
1:A:376:PHE:CD2	1:A:380:LEU:HD21	2.29	0.67
1:A:365:TRP:HH2	2:E:473:LEU:CD2	2.08	0.67
1:B:284:VAL:HG23	1:B:306:LYS:CG	2.27	0.64
1:B:224:ARG:HD2	2:E:484:GLU:O	1.99	0.63
2:E:489:PRO:C	2:E:491:PRO:HD3	2.21	0.61
1:A:356:LEU:HD23	1:B:356:LEU:HD23	1.84	0.59
2:E:486:LEU:HG	2:E:489:PRO:HD2	1.84	0.59
1:B:290:GLU:HG3	1:B:299:VAL:HG11	1.84	0.59
1:B:327:GLY:HA3	1:B:435:PRO:HG2	1.86	0.58
1:B:252:ASP:OD1	1:B:254:LYS:HB2	2.05	0.56
1:B:338:GLU:HG3	1:B:438:VAL:HG11	1.87	0.56
2:D:479:ARG:NH1	2:D:479:ARG:HB3	2.22	0.55
1:A:325:ARG:HB3	1:B:430:GLN:HB3	1.88	0.55
1:A:397:ILE:O	1:A:401:GLN:HG3	2.06	0.54
1:A:288:LEU:HB2	1:A:332:LEU:HD21	1.90	0.52
1:B:418:THR:HG23	1:B:421:LEU:H	1.73	0.52
2:E:488:ASP:N	2:E:489:PRO:HD3	2.24	0.52
1:B:404:ASN:ND2	2:D:480:ASP:OD1	2.41	0.52
2:E:489:PRO:CB	2:E:491:PRO:HD3	2.39	0.52
1:A:401:GLN:HG2	1:A:406:VAL:CG1	2.41	0.51
1:B:288:LEU:HB2	1:B:332:LEU:HD21	1.92	0.50
1:A:276:LEU:CD2	2:D:564:LYS:HD3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:THR:O	1:B:390:SER:HB2	2.12	0.49
1:A:427:LYS:O	1:A:428:SER:C	2.50	0.49
2:E:489:PRO:C	2:E:491:PRO:CD	2.80	0.49
2:E:485:PRO:O	2:E:486:LEU:CB	2.55	0.49
1:B:383:LYS:HG2	1:B:393:GLN:NE2	2.29	0.48
1:B:418:THR:CG2	1:B:421:LEU:H	2.26	0.48
1:A:217:MET:SD	2:D:544:LEU:HD11	2.55	0.47
1:A:370:LEU:O	1:A:374:ARG:HB2	2.14	0.47
2:E:473:LEU:HB3	2:E:475:VAL:H	1.79	0.47
2:E:486:LEU:HG	2:E:489:PRO:CD	2.45	0.46
1:B:208:TRP:CZ2	1:B:220:GLU:HB2	2.51	0.46
2:D:543:ASN:HB3	2:D:548:VAL:HG21	1.96	0.46
1:A:365:TRP:HH2	2:E:473:LEU:HD23	1.80	0.46
2:E:488:ASP:N	2:E:489:PRO:CD	2.79	0.46
1:B:403:LEU:O	1:B:404:ASN:HB2	2.15	0.46
1:A:409:TRP:HE3	1:A:414:VAL:HG21	1.81	0.45
1:B:200:ASP:OD1	1:B:200:ASP:N	2.45	0.45
1:A:226:HIS:ND1	2:D:544:LEU:HD13	2.31	0.45
1:B:254:LYS:HG3	1:B:281:GLU:HG3	1.98	0.45
1:A:395:ASP:OD1	2:E:473:LEU:HD22	2.16	0.45
1:B:439:ASP:OD2	1:B:441:VAL:HG22	2.17	0.45
1:A:411:GLY:O	1:A:412:GLN:HG2	2.17	0.44
1:A:376:PHE:CG	1:A:380:LEU:HD11	2.53	0.44
2:E:473:LEU:CG	2:E:474:ALA:N	2.59	0.44
1:A:224:ARG:HD2	2:D:484:GLU:O	2.17	0.43
1:A:225:PHE:CZ	1:A:229:GLN:HG3	2.53	0.43
2:E:488:ASP:O	2:E:489:PRO:C	2.56	0.43
1:A:411:GLY:C	1:A:412:GLN:HG2	2.39	0.43
1:A:324:GLN:O	1:A:325:ARG:HB2	2.18	0.42
1:A:376:PHE:CB	1:A:380:LEU:HD11	2.50	0.42
1:B:383:LYS:HE2	1:B:383:LYS:HB3	1.76	0.42
1:A:410:LYS:HD2	1:A:410:LYS:HA	1.32	0.42
1:A:276:LEU:HD21	2:D:564:LYS:HD3	2.02	0.41
1:B:374:ARG:NH2	1:B:426:LEU:HD13	2.35	0.41
1:A:325:ARG:HE	1:A:325:ARG:HA	1.85	0.41
1:A:389:THR:O	1:A:390:SER:HB2	2.20	0.41
1:B:177:LYS:HG2	1:B:203:LYS:O	2.20	0.41
1:B:430:GLN:HG3	1:B:430:GLN:H	1.41	0.41
2:E:553:HIS:HA	2:E:556:LEU:HD12	2.03	0.41
1:B:281:GLU:N	1:B:282:PRO:CD	2.83	0.41
1:A:197:PHE:HA	1:A:198:PRO:HD3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LYS:NZ	1:A:437:THR:HG21	2.37	0.40
2:E:473:LEU:CB	2:E:475:VAL:H	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	269/289 (93%)	261 (97%)	8 (3%)	0	100 100
1	B	263/289 (91%)	255 (97%)	8 (3%)	0	100 100
2	D	38/48 (79%)	37 (97%)	1 (3%)	0	100 100
2	E	40/48 (83%)	37 (92%)	2 (5%)	1 (2%)	5 1
All	All	610/674 (90%)	590 (97%)	19 (3%)	1 (0%)	47 39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	490	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	250/266 (94%)	240 (96%)	10 (4%)	31 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	247/266 (93%)	238 (96%)	9 (4%)	35 28
2	D	39/46 (85%)	33 (85%)	6 (15%)	2 0
2	E	44/46 (96%)	42 (96%)	2 (4%)	27 20
All	All	580/624 (93%)	553 (95%)	27 (5%)	26 18

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	LEU
1	A	277	TYR
1	A	359	LEU
1	A	374	ARG
1	A	380	LEU
1	A	409	TRP
1	A	410	LYS
1	A	423	GLU
1	A	432	LYS
1	A	449	LYS
1	B	200	ASP
1	B	277	TYR
1	B	359	LEU
1	B	390	SER
1	B	423	GLU
1	B	427	LYS
1	B	428	SER
1	B	430	GLN
1	B	444	LYS
2	D	479	ARG
2	D	483	VAL
2	D	487	ARG
2	D	488	ASP
2	D	547	SER
2	D	565	ARG
2	E	483	VAL
2	E	555	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	GLN

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Mol	Chain	Res	Type
1	B	183	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
1	ALY	A	274	1	10,11,12	0.56	0	7,12,14	1.15	0
1	ALY	B	274	1	10,11,12	0.66	0	7,12,14	0.89	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
1	ALY	A	274	1	-	0/9/10/12	-
1	ALY	B	274	1	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	271/289 (93%)	0.21	15 (5%)	25	27	19, 34, 63, 78	2 (0%)
1	B	267/289 (92%)	0.25	11 (4%)	37	40	22, 36, 62, 78	3 (1%)
2	D	42/48 (87%)	0.53	6 (14%)	2	2	26, 51, 64, 81	1 (2%)
2	E	46/48 (95%)	0.90	11 (23%)	0	0	25, 44, 89, 100	0
All	All	626/674 (92%)	0.30	43 (6%)	16	18	19, 37, 64, 100	6 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	408	TYR	7.3
2	E	490	ASN	6.2
1	A	409	TRP	5.9
2	E	491	PRO	5.3
2	E	492	SER	5.1
1	A	408	TYR	4.9
1	A	429	ALA	4.9
1	B	177	LYS	4.8
2	E	488	ASP	4.8
1	A	378	GLY	4.3
1	B	412	GLN	4.2
2	E	489	PRO	4.1
1	A	412	GLN	4.0
1	B	429	ALA	3.7
2	D	488	ASP	3.7
1	B	427	LYS	3.6
1	A	410	LYS	3.5
1	A	427	LYS	3.5
2	D	563	ARG	3.4
1	B	293	ARG	3.3
2	D	482	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	487	ARG	3.1
1	A	293	ARG	3.1
2	E	486	LEU	3.0
2	D	489	PRO	2.9
2	E	494	LEU	2.9
1	B	318	LEU	2.8
1	A	420	LYS	2.8
1	B	221	LYS	2.7
1	A	423	GLU	2.6
1	B	379	THR	2.6
2	E	565	ARG	2.5
1	A	356	LEU	2.4
1	A	276	LEU	2.3
2	E	495	LEU	2.3
1	A	377	ARG	2.3
1	A	414	VAL	2.2
1	A	231	GLN	2.2
2	E	484	GLU	2.1
2	D	565	ARG	2.1
1	B	420	LYS	2.1
1	B	356	LEU	2.0
2	E	473	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	ALY	A	274	12/13	0.91	0.16	22,25,30,30	0
1	ALY	B	274	12/13	0.92	0.16	21,23,28,29	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	ZN	A	501	1/1	0.98	0.10	41,41,41,41	0
3	ZN	B	501	1/1	0.99	0.09	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.