Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2024 – 11:49 AM EDT

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 (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:

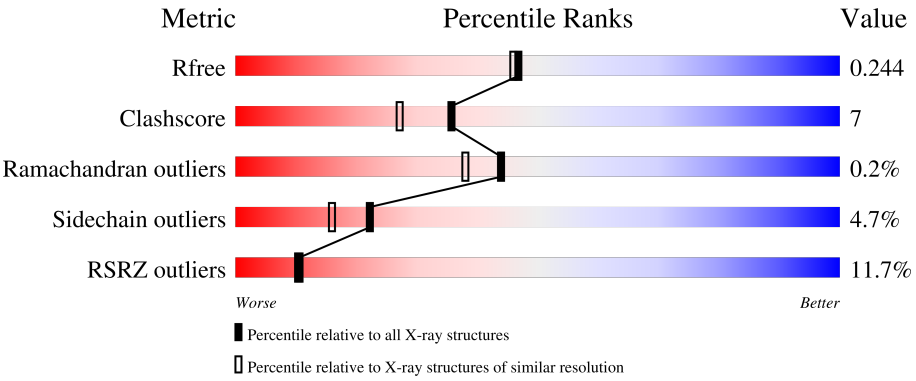
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (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 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	289	11% 80% 12% • 6%
1	B	289	9% 79% 13% • 7%
2	D	48	21% 63% 23% • 12%
2	E	48	15% 67% 29% •

2 Entry composition (i)

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	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

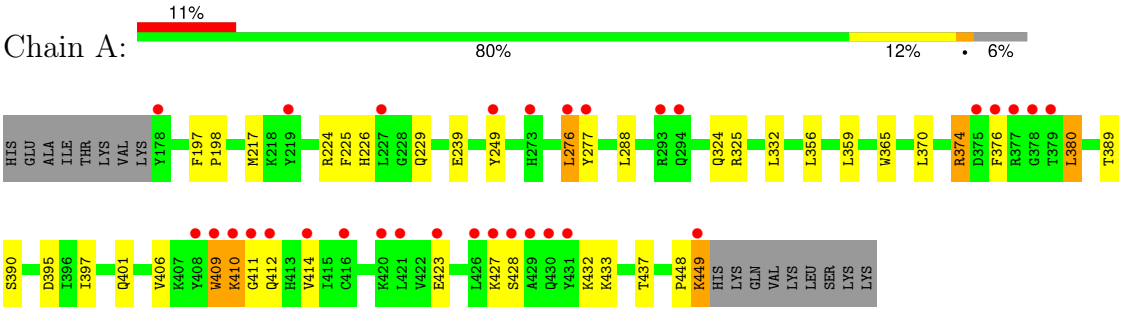
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	62	Total	O	0	0
			62	62		
4	D	5	Total	O	0	0
			5	5		
4	E	10	Total	O	0	0
			10	10		

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.

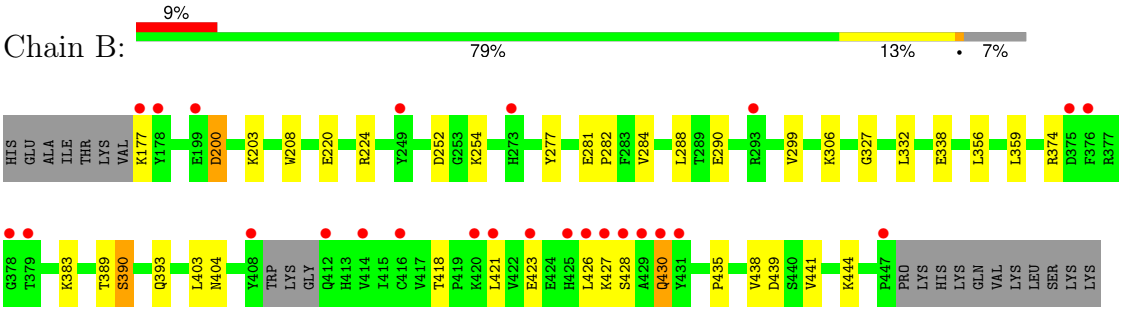
• Molecule 1: Histone acetyltransferase KAT8

Chain A:



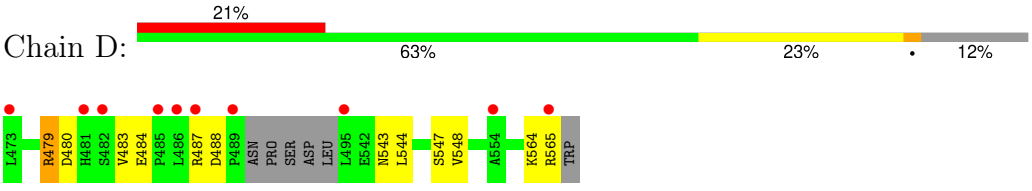
• Molecule 1: Histone acetyltransferase KAT8

Chain B:



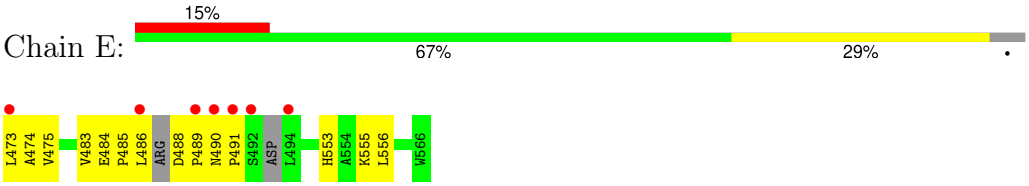
• Molecule 2: Male-specific lethal 1 homolog

Chain D:



• Molecule 2: Male-specific lethal 1 homolog

Chain E:



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 0.209 , 0.244	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 , 41.0	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

Continued on next page...

Continued from previous page...

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:HB3	2:D:479:ARG:NH1	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

Continued on next page...

Continued from previous page...

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:A:395:ASP:OD1	2:E:473:LEU:HD22	2.16	0.45
1:B:254:LYS:HG3	1:B:281:GLU:HG3	1.98	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:HA	1:A:410:LYS:HD2	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:HA	1:A:325:ARG:HE	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:H	1:B:430:GLN:HG3	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

Continued on next page...

Continued from previous page...

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%)	4 0
All	All	610/674 (90%)	590 (97%)	19 (3%)	1 (0%)	44 38

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%)	27 21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	247/266 (93%)	238 (96%)	9 (4%)	30 25
2	D	39/46 (85%)	33 (85%)	6 (15%)	2 0
2	E	44/46 (96%)	42 (96%)	2 (4%)	23 17
All	All	580/624 (93%)	553 (95%)	27 (5%)	22 16

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

Sometimes 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

Continued on next page...

Continued from previous page...

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	B	274	1	10,11,12	0.64	0	7,12,14	0.93	0
1	ALY	A	274	1	10,11,12	0.58	0	7,12,14	1.18	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	B	274	1	-	0/9/10/12	-
1	ALY	A	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 oligosaccharides 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%)	0.40	31 (11%) 11 11	19, 34, 63, 78	2 (0%)
1	B	267/289 (92%)	0.45	25 (9%) 15 17	22, 36, 62, 78	2 (0%)
2	D	42/48 (87%)	1.14	10 (23%) 2 1	26, 51, 64, 81	1 (2%)
2	E	46/48 (95%)	1.22	7 (15%) 6 6	25, 44, 89, 100	0
All	All	626/674 (92%)	0.53	73 (11%) 10 10	19, 37, 64, 100	5 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	408	TYR	7.0
2	E	491	PRO	5.7
2	E	486	LEU	5.5
2	E	492	SER	5.4
1	B	429	ALA	4.8
2	D	489	PRO	4.8
2	E	489	PRO	4.8
1	A	409	TRP	4.8
1	A	408	TYR	4.6
1	A	429	ALA	4.5
1	A	378	GLY	4.5
1	B	412	GLN	4.1
2	E	473	LEU	4.0
1	A	276	LEU	3.8
1	A	178	TYR	3.7
1	B	431	TYR	3.6
2	D	495	LEU	3.5
1	A	410	LYS	3.5
1	A	431	TYR	3.3
1	A	414	VAL	3.2
1	B	426	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	379	THR	3.1
2	D	486	LEU	3.1
1	B	273	HIS	3.0
2	E	494	LEU	3.0
1	A	423	GLU	3.0
1	B	177	LYS	3.0
1	B	425	HIS	3.0
1	B	178	TYR	2.9
1	A	428	SER	2.9
1	A	427	LYS	2.9
1	B	375	ASP	2.8
1	A	376	PHE	2.8
1	B	428	SER	2.8
1	B	379	THR	2.8
1	B	430	GLN	2.7
1	A	375	ASP	2.7
1	B	423	GLU	2.7
1	A	277	TYR	2.6
1	B	414	VAL	2.6
1	A	219	TYR	2.6
2	D	487	ARG	2.6
1	A	426	LEU	2.6
1	B	421	LEU	2.6
1	A	249	TYR	2.5
1	A	421	LEU	2.5
1	A	377	ARG	2.5
1	A	294	GLN	2.5
1	B	427	LYS	2.4
1	A	412	GLN	2.4
1	A	273	HIS	2.4
1	A	449	LYS	2.4
2	D	481	HIS	2.4
2	D	565	ARG	2.4
1	A	293	ARG	2.3
2	D	482	SER	2.3
1	A	430	GLN	2.3
1	B	376	PHE	2.3
1	B	447	PRO	2.3
1	A	411	GLY	2.3
1	A	227	LEU	2.2
1	A	420	LYS	2.2
1	B	378	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	554	ALA	2.2
2	D	485	PRO	2.2
2	D	473	LEU	2.1
1	B	249	TYR	2.1
1	B	420	LYS	2.1
2	E	490	ASN	2.1
1	B	199	GLU	2.1
1	A	416	CYS	2.1
1	B	416	CYS	2.1
1	B	293	ARG	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	0.87	0.11	22,25,30,30	0
1	ALY	B	274	12/13	0.91	0.10	21,23,28,29	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	ZN	A	501	1/1	0.99	0.03	41,41,41,41	0
3	ZN	B	501	1/1	0.99	0.02	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.