Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 08:36 am GMT

PDB ID	:	4BZ8
Title	:	Crystal structure of Schistosoma mansoni HDAC8 complexed with J1038
Authors	:	Marek, M.; Romier, C.
Deposited on	:	2013-07-24
Resolution	:	2.21 Å(reported)

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

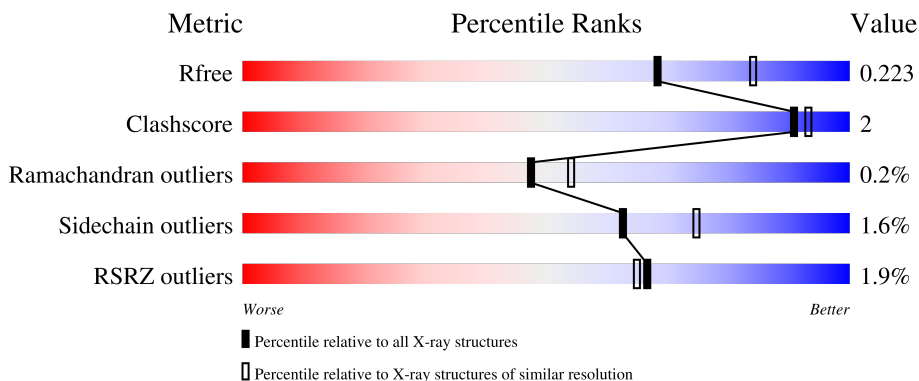|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.21 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	Percentile Ranks	Value
Rfree		0.223
Clashscore		2
Ramachandran outliers		0.2%
Sidechain outliers		1.6%
RSRZ outliers		1.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	446	3% / 85% · 12%
1	B	446	% / 89% · 7%
1	C	446	87% 5% 7%
1	D	446	2% / 83% · · 12%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 13510 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 DEACETYLASE 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total 3130	C 2017	N 524	O 575	S 14	0	0	0
1	B	415	Total 3313	C 2135	N 555	O 608	S 15	0	0	0
1	C	413	Total 3295	C 2124	N 551	O 604	S 16	0	0	0
1	D	394	Total 3145	C 2026	N 526	O 579	S 14	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	GLY	-	expression tag	UNP A5H660
A	442	SER	-	expression tag	UNP A5H660
A	443	LEU	-	expression tag	UNP A5H660
A	444	VAL	-	expression tag	UNP A5H660
A	445	PRO	-	expression tag	UNP A5H660
A	446	ARG	-	expression tag	UNP A5H660
B	441	GLY	-	expression tag	UNP A5H660
B	442	SER	-	expression tag	UNP A5H660
B	443	LEU	-	expression tag	UNP A5H660
B	444	VAL	-	expression tag	UNP A5H660
B	445	PRO	-	expression tag	UNP A5H660
B	446	ARG	-	expression tag	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is (2R)-2-methyl-3-oxo-4H-1,4-benzothiazine-6-carbohydroxamic acid (three-letter code: J38) (formula: $C_{10}H_{10}N_2O_3S$).

J38

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
4	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
4	D	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	132	Total	O	0	0
			132	132		
5	C	157	Total	O	0	0
			157	157		
5	D	131	Total	O	0	0
			131	131		

3 Residue-property plots ⓘ

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.
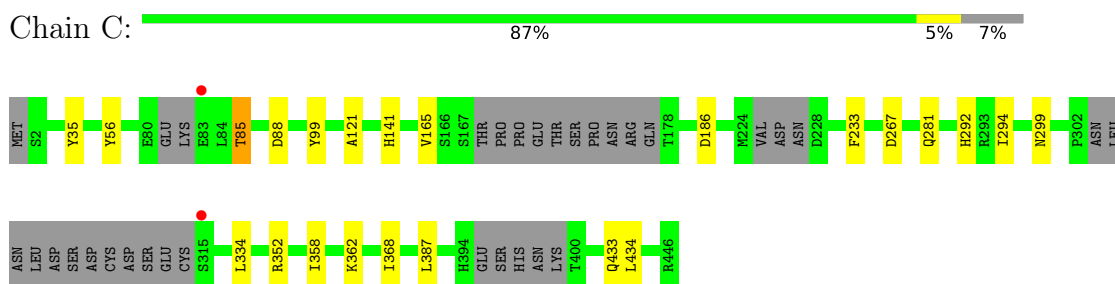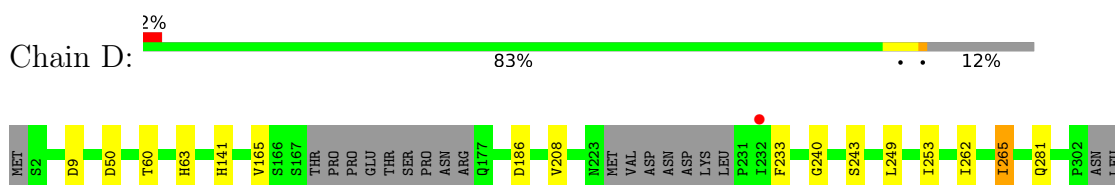
- Molecule 1: HISTONE DEACETYLASE 8
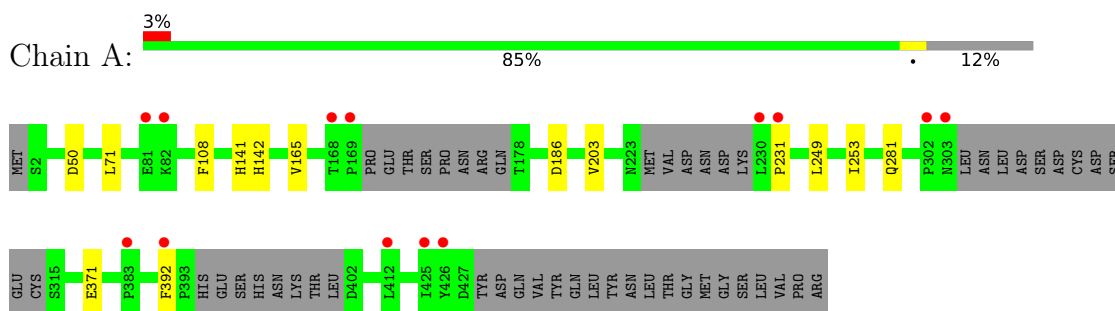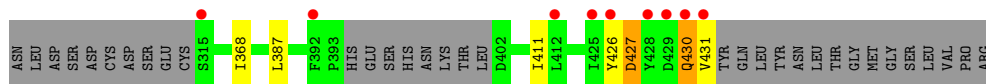

- Molecule 1: HISTONE DEACETYLASE 8
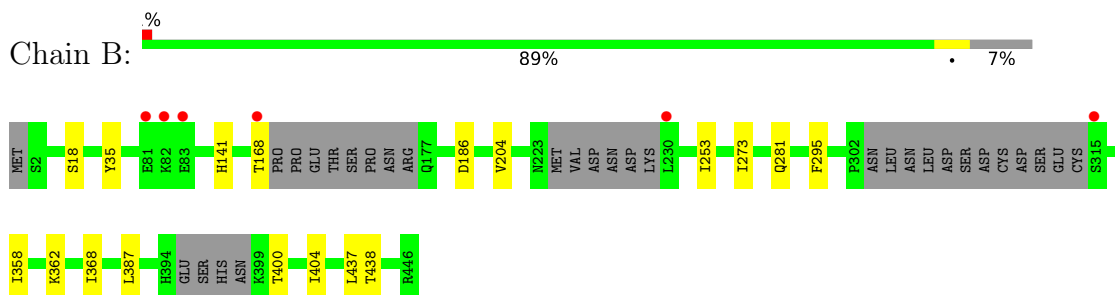
- Molecule 1: HISTONE DEACETYLASE 8

- Molecule 1: HISTONE DEACETYLASE 8

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.66Å 70.72Å 98.39Å 77.98° 75.51° 85.80°	Depositor
Resolution (Å)	32.36 – 2.21 49.76 – 2.21	Depositor EDS
% Data completeness (in resolution range)	93.2 (32.36-2.21) 92.8 (49.76-2.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.178 , 0.222 0.181 , 0.223	Depositor DCC
R_{free} test set	4297 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13510	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: J38, K, ZN

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	0.49	0/3218	0.61	0/4378
1	B	0.49	0/3405	0.60	0/4631
1	C	0.50	0/3386	0.61	0/4604
1	D	0.47	0/3233	0.62	0/4396
All	All	0.49	0/13242	0.61	0/18009

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	3130	0	3031	6	0
1	B	3313	0	3216	9	0
1	C	3295	0	3193	14	0
1	D	3145	0	3039	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	16	0	10	1	0
4	B	16	0	10	1	0
4	C	16	0	9	1	0
4	D	16	0	10	0	0
5	A	131	0	0	0	0
5	B	132	0	0	0	0
5	C	157	0	0	0	0
5	D	131	0	0	0	0
All	All	13510	0	12518	42	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 2.

All (42) 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:C:368:ILE:HG21	1:C:387:LEU:CD2	2.15	0.77
1:C:121:ALA:HB1	1:C:334:LEU:HD11	1.70	0.73
1:C:368:ILE:HG21	1:C:387:LEU:HD22	1.69	0.73
1:B:368:ILE:HG21	1:B:387:LEU:HD22	1.73	0.71
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.26	0.70
1:B:368:ILE:HG21	1:B:387:LEU:CD2	2.23	0.68
1:C:368:ILE:CG2	1:C:387:LEU:HD22	2.25	0.67
1:D:265:ILE:HD12	1:D:411:ILE:HG21	1.79	0.63
1:C:292:HIS:HB3	1:C:294:ILE:HD12	1.81	0.62
1:B:368:ILE:CG2	1:B:387:LEU:HD22	2.29	0.62
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.35	0.61
1:C:186:ASP:HB2	1:C:281:GLN:OE1	2.05	0.57
1:D:426:TYR:O	1:D:427:ASP:HB2	2.07	0.55
4:C:700:J38:O16	1:D:50:ASP:HB3	2.09	0.52
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.09	0.52
1:C:85:THR:HG22	1:C:88:ASP:H	1.74	0.52
1:C:368:ILE:CG2	1:C:387:LEU:CD2	2.84	0.52
1:D:249:LEU:HD13	1:D:253:ILE:HD13	1.92	0.52
1:A:249:LEU:HD13	1:A:253:ILE:HD13	1.91	0.51
1:C:121:ALA:CB	1:C:334:LEU:HD11	2.41	0.50
1:B:186:ASP:HB2	1:B:281:GLN:OE1	2.14	0.48
1:D:60:THR:HA	1:D:63:HIS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:ILE:CG2	1:D:387:LEU:HD22	2.44	0.47
1:C:294:ILE:HD11	1:D:50:ASP:O	2.15	0.46
1:B:358:ILE:HG23	1:B:362:LYS:HD3	1.97	0.46
1:C:299:ASN:O	1:C:352:ARG:HD2	2.17	0.44
1:A:186:ASP:HB2	1:A:281:GLN:OE1	2.17	0.44
1:C:358:ILE:HG23	1:C:362:LYS:HD3	1.99	0.44
1:A:50:ASP:HB3	4:B:700:J38:O16	2.17	0.44
1:A:71:LEU:HG	1:A:108:PHE:HD1	1.83	0.44
1:B:368:ILE:CG2	1:B:387:LEU:CD2	2.92	0.43
1:C:267:ASP:HB3	1:C:434:LEU:HD11	2.00	0.43
1:D:430:GLN:HG2	1:D:431:VAL:N	2.34	0.43
1:B:253:ILE:HG22	1:B:295:PHE:CD1	2.54	0.43
1:A:165:VAL:HG11	1:A:203:VAL:CG2	2.50	0.42
1:D:208:VAL:HG11	1:D:262:ILE:HD12	2.01	0.41
1:B:204:VAL:HG21	1:B:273:ILE:HG12	2.03	0.41
1:A:142:HIS:NE2	4:A:700:J38:N10	2.67	0.41
1:D:265:ILE:HD12	1:D:411:ILE:CG2	2.49	0.41
1:D:430:GLN:HG2	1:D:431:VAL:H	1.87	0.40
1:D:368:ILE:HG22	1:D:387:LEU:HD22	2.03	0.40
1:D:240:GLY:O	1:D:243:SER:OG	2.39	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	383/446 (86%)	375 (98%)	8 (2%)	0	100	100
1	B	405/446 (91%)	397 (98%)	8 (2%)	0	100	100
1	C	401/446 (90%)	393 (98%)	7 (2%)	1 (0%)	47	54
1	D	384/446 (86%)	369 (96%)	13 (3%)	2 (0%)	29	30
All	All	1573/1784 (88%)	1534 (98%)	36 (2%)	3 (0%)	47	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	427	ASP
1	C	99	TYR
1	D	430	GLN

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	340/391 (87%)	336 (99%)	4 (1%)	71	82
1	B	360/391 (92%)	353 (98%)	7 (2%)	57	69
1	C	358/391 (92%)	352 (98%)	6 (2%)	60	73
1	D	341/391 (87%)	336 (98%)	5 (2%)	65	76
All	All	1399/1564 (90%)	1377 (98%)	22 (2%)	62	75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	231	PRO
1	A	371	GLU
1	A	392	PHE
1	B	18	SER
1	B	141	HIS
1	B	168	THR
1	B	400	THR
1	B	404	ILE
1	B	437	LEU
1	B	438	THR
1	C	56	TYR
1	C	85	THR
1	C	141	HIS
1	C	165	VAL
1	C	233	PHE
1	C	433	GLN

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Mol	Chain	Res	Type
1	D	9	ASP
1	D	141	HIS
1	D	165	VAL
1	D	233	PHE
1	D	265	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	394	HIS

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 ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 12 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	J38	D	700	2	16,17,17	6.53	10 (62%)	20,24,24	1.47	4 (20%)
4	J38	B	700	2	16,17,17	6.38	10 (62%)	20,24,24	1.47	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	J38	A	700	2	16,17,17	6.48	10 (62%)	20,24,24	1.25	4 (20%)
4	J38	C	700	2	16,17,17	6.45	10 (62%)	20,24,24	1.44	5 (25%)

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	J38	D	700	2	-	0/6/18/18	0/2/2/2
4	J38	B	700	2	-	0/6/18/18	0/2/2/2
4	J38	A	700	2	-	0/6/18/18	0/2/2/2
4	J38	C	700	2	-	0/6/18/18	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	700	J38	C02-S03	-14.90	1.68	1.82
4	C	700	J38	C02-S03	-14.82	1.68	1.82
4	A	700	J38	C02-S03	-14.74	1.68	1.82
4	B	700	J38	C02-S03	-14.50	1.69	1.82
4	D	700	J38	C15-N14	13.48	1.50	1.34
4	A	700	J38	C15-N14	13.30	1.50	1.34
4	C	700	J38	C15-N14	13.24	1.50	1.34
4	B	700	J38	C15-N14	13.04	1.49	1.34
4	A	700	J38	C08-N10	9.02	1.44	1.32
4	C	700	J38	C08-N10	8.76	1.44	1.32
4	B	700	J38	C08-N10	8.62	1.43	1.32
4	D	700	J38	C08-N10	8.54	1.43	1.32
4	D	700	J38	C13-C04	8.20	1.53	1.40
4	A	700	J38	C13-C04	8.13	1.53	1.40
4	C	700	J38	C13-C04	8.00	1.53	1.40
4	B	700	J38	C13-C04	7.99	1.53	1.40
4	D	700	J38	C13-N14	7.58	1.52	1.39
4	B	700	J38	C13-N14	7.50	1.52	1.39
4	C	700	J38	C13-N14	7.42	1.52	1.39
4	A	700	J38	C13-N14	7.42	1.52	1.39
4	D	700	J38	C06-C07	5.18	1.48	1.39
4	B	700	J38	C06-C07	5.14	1.48	1.39
4	C	700	J38	C06-C07	5.09	1.48	1.39
4	A	700	J38	C06-C07	4.89	1.47	1.39
4	D	700	J38	C04-S03	-4.36	1.70	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	J38	C04-S03	-4.22	1.70	1.76
4	B	700	J38	C04-S03	-3.99	1.70	1.76
4	C	700	J38	C04-S03	-3.80	1.71	1.76
4	D	700	J38	O11-N10	-3.63	1.30	1.40
4	B	700	J38	O11-N10	-3.49	1.31	1.40
4	C	700	J38	O11-N10	-3.48	1.31	1.40
4	A	700	J38	O11-N10	-3.47	1.31	1.40
4	D	700	J38	C12-C07	3.42	1.44	1.39
4	A	700	J38	C12-C07	3.40	1.44	1.39
4	B	700	J38	C06-C05	3.29	1.44	1.38
4	C	700	J38	C12-C07	3.29	1.44	1.39
4	B	700	J38	C12-C07	3.28	1.44	1.39
4	D	700	J38	C06-C05	3.05	1.44	1.38
4	C	700	J38	C06-C05	3.04	1.44	1.38
4	A	700	J38	C06-C05	2.87	1.44	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	700	J38	C07-C08-N10	3.54	121.84	116.16
4	B	700	J38	C07-C08-N10	3.41	121.63	116.16
4	C	700	J38	C07-C08-N10	3.09	121.11	116.16
4	A	700	J38	O16-C15-N14	-2.95	118.65	122.11
4	D	700	J38	C01-C02-C15	-2.73	109.27	112.03
4	B	700	J38	O09-C08-N10	-2.69	117.91	122.94
4	D	700	J38	O09-C08-N10	-2.68	117.93	122.94
4	B	700	J38	O16-C15-N14	-2.67	118.98	122.11
4	C	700	J38	O09-C08-N10	-2.59	118.10	122.94
4	C	700	J38	C01-C02-C15	-2.57	109.43	112.03
4	C	700	J38	O16-C15-N14	-2.56	119.10	122.11
4	A	700	J38	C07-C08-N10	2.53	120.22	116.16
4	B	700	J38	C04-C13-N14	-2.26	118.07	120.66
4	A	700	J38	C04-C13-N14	-2.19	118.15	120.66
4	D	700	J38	C04-C13-N14	-2.11	118.23	120.66
4	C	700	J38	C04-C13-N14	-2.10	118.25	120.66
4	A	700	J38	O09-C08-N10	-2.09	119.04	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	700	J38	1	0
4	A	700	J38	1	0
4	C	700	J38	1	0

5.7 Other polymers ⓘ

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, 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	393/446 (88%)	-0.24	13 (3%) 46	44	12, 24, 51, 96	0
1	B	415/446 (93%)	-0.39	6 (1%) 75	73	10, 20, 45, 75	0
1	C	413/446 (92%)	-0.44	2 (0%) 91	90	9, 20, 41, 79	0
1	D	394/446 (88%)	-0.26	10 (2%) 57	55	12, 24, 52, 99	0
All	All	1615/1784 (90%)	-0.33	31 (1%) 66	65	9, 22, 48, 99	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	392	PHE	4.6
1	D	315	SER	4.3
1	A	425	ILE	3.8
1	D	428	TYR	3.8
1	A	426	TYR	3.5
1	A	169	PRO	3.3
1	D	392	PHE	3.3
1	B	83	GLU	3.1
1	D	425	ILE	3.1
1	B	81	GLU	3.1
1	B	315	SER	3.0
1	A	81	GLU	3.0
1	A	168	THR	3.0
1	A	230	LEU	2.9
1	A	231	PRO	2.8
1	B	168	THR	2.8
1	D	431	VAL	2.8
1	D	430	GLN	2.7
1	A	82	LYS	2.6
1	A	303	ASN	2.6
1	B	230	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	426	TYR	2.5
1	D	232	ILE	2.5
1	A	412	LEU	2.4
1	D	429	ASP	2.4
1	D	412	LEU	2.3
1	A	302	PRO	2.2
1	C	83	GLU	2.2
1	A	383	PRO	2.2
1	C	315	SER	2.1
1	B	82	LYS	2.1

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 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, 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	J38	A	700	16/16	0.85	0.22	51,53,54,54	0
4	J38	D	700	16/16	0.88	0.24	66,67,69,69	0
4	J38	B	700	16/16	0.90	0.19	48,50,54,54	0
4	J38	C	700	16/16	0.91	0.17	43,50,56,56	0
3	K	A	600	1/1	0.97	0.06	30,30,30,30	0
3	K	C	601	1/1	0.97	0.06	31,31,31,31	0
3	K	D	600	1/1	0.98	0.08	30,30,30,30	0
3	K	B	600	1/1	0.99	0.09	29,29,29,29	0
3	K	D	601	1/1	0.99	0.07	16,16,16,16	0
2	ZN	C	500	1/1	1.00	0.07	21,21,21,21	0
2	ZN	D	500	1/1	1.00	0.07	22,22,22,22	0
2	ZN	A	500	1/1	1.00	0.06	22,22,22,22	0
3	K	A	601	1/1	1.00	0.07	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	500	1/1	1.00	0.05	19,19,19,19	0
3	K	B	601	1/1	1.00	0.07	11,11,11,11	0
3	K	C	600	1/1	1.00	0.06	12,12,12,12	0

6.5 Other polymers ⓘ

There are no such residues in this entry.