



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:45 AM GMT

PDB ID : 3C10  
Title : Crystal structure of catalytic domain of human histone deacetylase HDAC7 in complex with Trichostatin A (TSA)  
Authors : Min, J.; Schuetz, A.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)  
Deposited on : 2008-01-21  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



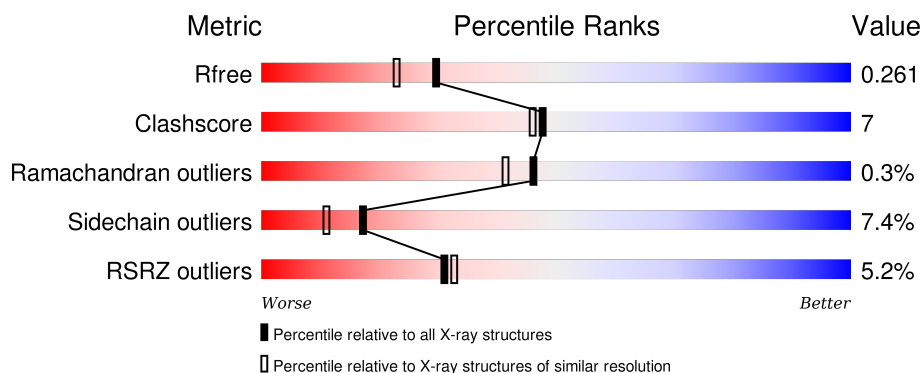
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	423	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	423	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>17%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	423	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>15%</div> <div>•</div> <div>15%</div> </div> </div>

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	TSN	A	301	-	-	-	X



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8961 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 7a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2902	1819	524	540	19			
1	B	368	Total	C	N	O	S	0	0	0
			2794	1751	506	518	19			
1	C	359	Total	C	N	O	S	0	0	0
			2728	1706	494	510	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	-	EXPRESSION TAG	UNP Q8WUI4
B	481	GLY	-	EXPRESSION TAG	UNP Q8WUI4
C	481	GLY	-	EXPRESSION TAG	UNP Q8WUI4

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

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

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

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

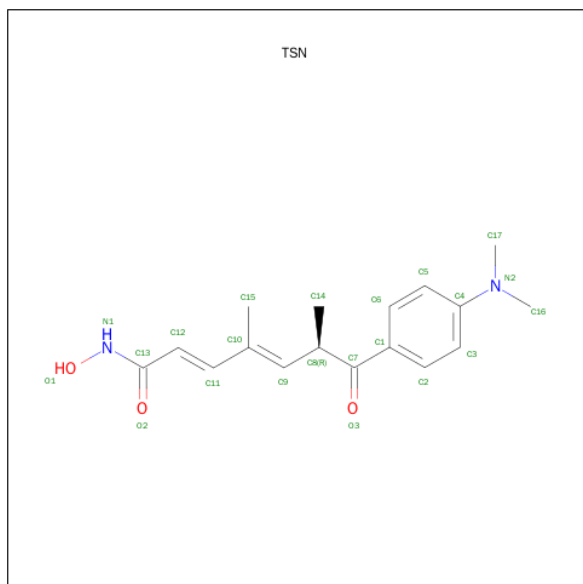
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	K	0	0
			2	2		

- Molecule 4 is TRICHOSTATIN A (three-letter code: TSN) (formula: C<sub>17</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	17	2	3		
4	B	1	Total	C	N	O	0	0
			22	17	2	3		
4	C	1	Total	C	N	O	0	0
			22	17	2	3		

- Molecule 5 is water.

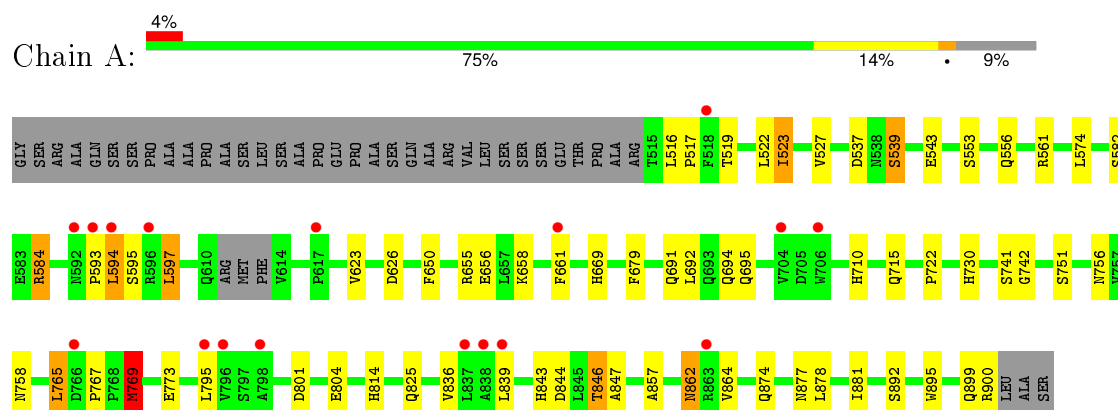
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total	O	0	0
			170	170		
5	B	159	Total	O	0	0
			159	159		
5	C	130	Total	O	0	0
			130	130		



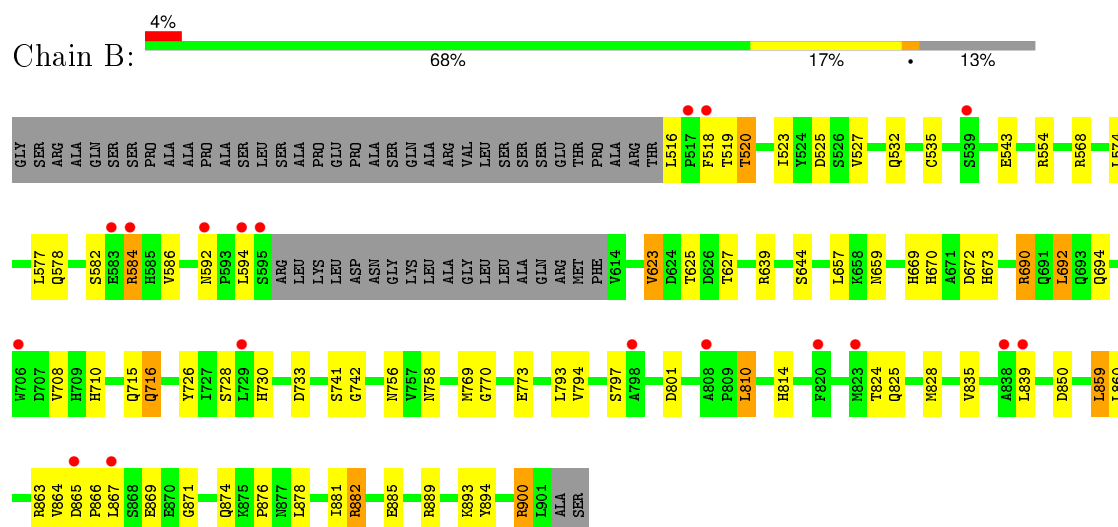
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

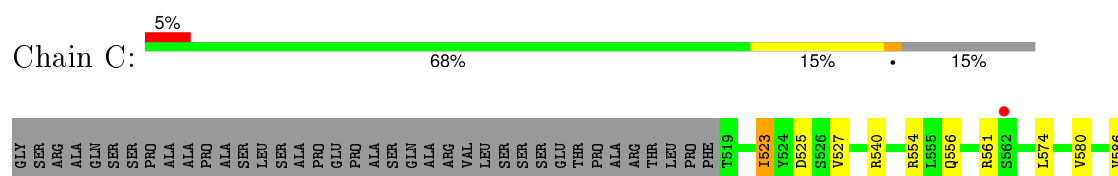
#### • Molecule 1: Histone deacetylase 7a



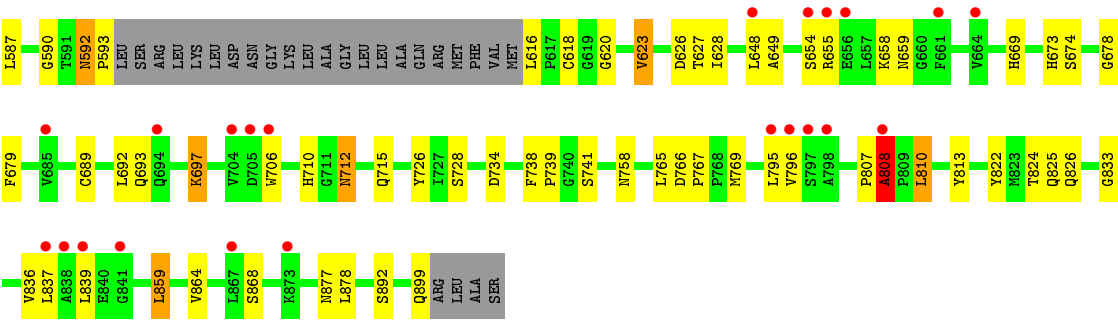
#### • Molecule 1: Histone deacetylase 7a



#### • Molecule 1: Histone deacetylase 7a









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.83Å 81.83Å 148.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.42 – 2.00 34.47 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.42-2.00) 97.5 (34.47-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.263 0.199 , 0.261	Depositor DCC
$R_{free}$ test set	3651 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
Estimated twinning fraction	0.006 for -h,-k,l 0.035 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 73442 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TSN, ZN, K

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	0.85	1/2970 (0.0%)	0.83	3/4029 (0.1%)
1	B	0.86	0/2862	0.88	3/3883 (0.1%)
1	C	0.72	0/2794	0.76	0/3791
All	All	0.81	1/8626 (0.0%)	0.82	6/11703 (0.1%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	VAL	CB-CG2	5.18	1.63	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	690	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	769	MET	CG-SD-CE	6.09	109.94	100.20
1	A	801	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	801	ASP	CB-CG-OD1	5.55	123.29	118.30
1	B	801	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	692	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	C	808	ALA	Peptide

## 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	2902	0	2803	37	0
1	B	2794	0	2688	44	0
1	C	2728	0	2617	42	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	1	0
4	A	22	0	21	0	0
4	B	22	0	21	2	0
4	C	22	0	21	1	0
5	A	170	0	0	4	0
5	B	159	0	0	7	0
5	C	130	0	0	2	0
All	All	8961	0	8171	123	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 (123) 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:B:672:ASP:HB2	1:B:716:GLN:NE2	1.83	0.92
1:B:769:MET:HE1	5:B:1023:HOH:O	1.70	0.92
1:B:825:GLN:HE22	1:B:864:VAL:H	1.19	0.90
1:B:672:ASP:HB2	1:B:716:GLN:HE21	1.33	0.89
1:C:833:GLY:O	5:C:938:HOH:O	1.95	0.83
1:C:892:SER:O	1:C:899:GLN:HG3	1.79	0.82
1:B:769:MET:CE	5:B:1023:HOH:O	2.29	0.79
1:C:807:PRO:O	1:C:808:ALA:C	2.21	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:THR:O	1:A:658:LYS:N	2.16	0.76
1:B:733:ASP:OD1	5:B:1035:HOH:O	2.04	0.76
1:B:670:HIS:HE2	4:B:301:TSN:HN1	1.33	0.76
1:A:804:GLU:OE1	1:A:814:HIS:HD2	1.69	0.76
1:C:592:ASN:HB2	1:C:593:PRO:HA	1.68	0.75
1:B:520:THR:HB	1:B:659:ASN:OD1	1.88	0.73
1:C:715:GLN:HE22	1:C:758:ASN:HD21	1.33	0.73
1:B:673:HIS:H	1:B:716:GLN:HE22	1.36	0.71
1:A:825:GLN:HE22	1:A:864:VAL:H	1.38	0.70
1:B:525:ASP:OD2	1:B:527:VAL:HG23	1.92	0.70
1:B:554:ARG:NH2	1:B:850:ASP:OD1	2.23	0.69
1:A:715:GLN:HE22	1:A:758:ASN:HD21	1.43	0.67
1:B:825:GLN:NE2	1:B:864:VAL:H	1.92	0.67
1:C:654:SER:O	1:C:655:ARG:HB2	1.94	0.66
1:A:900:ARG:NE	5:A:270:HOH:O	2.32	0.62
1:A:722:PRO:HD3	1:A:751:SER:HB3	1.80	0.62
1:C:825:GLN:HE22	1:C:864:VAL:H	1.49	0.60
3:C:202:K:K	5:C:906:HOH:O	2.11	0.60
1:A:710:HIS:HD2	1:A:741:SER:OG	1.85	0.59
1:C:580:VAL:O	1:C:673:HIS:HD2	1.85	0.59
1:B:876:PRO:HG2	1:B:881:ILE:HD11	1.83	0.59
1:A:825:GLN:NE2	1:A:864:VAL:H	2.01	0.59
1:B:715:GLN:HE22	1:B:758:ASN:HD21	1.48	0.58
1:A:556:GLN:HB2	1:A:561:ARG:CZ	2.34	0.58
1:B:584:ARG:H	1:B:584:ARG:HD3	1.68	0.57
1:C:710:HIS:HD2	1:C:741:SER:OG	1.87	0.57
1:C:825:GLN:NE2	1:C:864:VAL:H	2.02	0.57
1:C:623:VAL:HG22	1:C:627:THR:HB	1.86	0.57
1:A:804:GLU:OE1	1:A:814:HIS:CD2	2.55	0.57
1:C:810:LEU:HG	4:C:301:TSN:H21	1.88	0.56
1:A:650:PHE:HE1	1:A:691:GLN:HB3	1.71	0.56
1:A:517:PRO:HG2	1:C:587:LEU:HD11	1.87	0.56
1:C:616:LEU:HB2	1:C:620:GLY:O	2.06	0.55
1:A:857:ALA:O	1:A:862:ASN:HB3	2.07	0.54
1:A:523:ILE:O	1:A:523:ILE:HG22	2.07	0.54
1:C:715:GLN:NE2	1:C:758:ASN:HD21	2.05	0.54
1:A:626:ASP:HB3	1:A:679:PHE:CE1	2.43	0.54
1:B:810:LEU:HD12	5:B:1038:HOH:O	2.07	0.53
1:C:689:CYS:O	1:C:693:GLN:HG3	2.09	0.53
1:C:795:LEU:HD23	1:C:836:VAL:HB	1.91	0.52
1:B:670:HIS:CD2	4:B:301:TSN:HN1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:PHE:CE1	1:A:691:GLN:HB3	2.46	0.51
1:C:540:ARG:HE	1:C:618:CYS:HB3	1.76	0.50
1:C:592:ASN:CB	1:C:593:PRO:HA	2.38	0.50
1:C:523:ILE:HG13	1:C:648:LEU:HD22	1.92	0.50
1:B:582:SER:HB3	1:B:673:HIS:CE1	2.48	0.49
1:C:712:ASN:H	1:C:712:ASN:HD22	1.58	0.49
1:B:715:GLN:NE2	1:B:758:ASN:HD21	2.08	0.49
1:C:796:VAL:HB	1:C:837:LEU:HD22	1.94	0.49
1:B:710:HIS:HD2	1:B:741:SER:OG	1.95	0.48
1:B:520:THR:HG23	1:B:860:LEU:HD23	1.94	0.48
1:B:523:ILE:HG21	1:B:644:SER:HB3	1.95	0.48
1:A:844:ASP:HB3	1:A:847:ALA:HB3	1.94	0.48
1:B:690:ARG:O	1:B:694:GLN:HG3	2.13	0.48
1:B:824:THR:O	1:B:828:MET:HG3	2.13	0.48
1:A:650:PHE:HE2	1:A:695:GLN:HG2	1.79	0.47
1:B:710:HIS:CE1	1:B:715:GLN:NE2	2.83	0.47
1:C:525:ASP:OD2	1:C:527:VAL:HG23	2.15	0.47
1:B:578:GLN:HG3	1:B:586:VAL:HG21	1.97	0.47
1:C:649:ALA:HA	1:C:836:VAL:HG21	1.96	0.47
1:B:871:GLY:HA2	1:B:874:GLN:HG2	1.96	0.46
1:C:726:TYR:CZ	1:C:728:SER:HB2	2.49	0.46
1:C:892:SER:O	1:C:899:GLN:CG	2.58	0.46
1:C:655:ARG:HD3	1:C:655:ARG:N	2.31	0.46
1:C:769:MET:HB2	1:C:813:TYR:CD2	2.51	0.46
1:A:595:SER:HB3	1:A:597:LEU:HB2	1.97	0.46
1:C:556:GLN:HB2	1:C:561:ARG:NH1	2.30	0.46
1:A:522:LEU:HD23	1:A:661:PHE:HB3	1.98	0.46
1:B:794:VAL:HB	1:B:835:VAL:HG22	1.98	0.46
1:C:658:LYS:HD3	1:C:659:ASN:ND2	2.31	0.46
1:A:556:GLN:HB2	1:A:561:ARG:NE	2.30	0.45
1:A:795:LEU:HD23	1:A:836:VAL:HB	1.98	0.45
1:C:592:ASN:CB	1:C:593:PRO:CA	2.94	0.45
1:A:846:THR:HG23	5:A:468:HOH:O	2.16	0.45
1:A:553:SER:HA	1:A:561:ARG:HH11	1.82	0.45
1:B:863:ARG:HD2	5:B:1060:HOH:O	2.16	0.45
1:C:626:ASP:HB3	1:C:679:PHE:CE1	2.52	0.45
1:A:730:HIS:HE1	1:A:742:GLY:O	2.01	0.44
1:A:895:TRP:O	1:A:899:GLN:HG3	2.17	0.44
1:A:769:MET:SD	1:A:773:GLU:HG2	2.58	0.44
1:C:586:VAL:O	1:C:590:GLY:HA3	2.16	0.44
1:A:892:SER:O	1:A:899:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:738:PHE:HA	1:C:739:PRO:HA	1.76	0.44
1:C:822:TYR:O	1:C:826:GLN:HG3	2.18	0.44
1:C:678:GLY:O	1:C:679:PHE:HB2	2.18	0.44
1:C:710:HIS:CE1	1:C:715:GLN:NE2	2.86	0.43
1:B:885:GLU:CD	1:B:900:ARG:HH22	2.22	0.43
1:B:866:PRO:O	1:B:867:LEU:CB	2.67	0.43
1:A:582:SER:OG	1:A:584:ARG:HD3	2.19	0.43
1:A:900:ARG:NH2	5:A:270:HOH:O	2.50	0.43
1:B:623:VAL:HG22	1:B:627:THR:HB	2.01	0.43
1:B:728:SER:OG	1:B:730:HIS:HD2	2.01	0.43
1:A:593:PRO:HA	1:A:594:LEU:HA	1.72	0.43
1:B:726:TYR:HD2	1:B:756:ASN:ND2	2.17	0.42
1:B:577:LEU:HD11	1:B:639:ARG:HG2	2.00	0.42
1:B:592:ASN:HD22	1:B:594:LEU:H	1.66	0.42
1:C:767:PRO:HG2	1:C:877:ASN:HB2	2.01	0.42
1:A:756:ASN:ND2	5:A:34:HOH:O	2.44	0.42
1:B:824:THR:CG2	1:B:859:LEU:HD13	2.49	0.42
1:B:814:HIS:CD2	5:B:971:HOH:O	2.72	0.42
1:C:766:ASP:HA	1:C:767:PRO:C	2.39	0.42
1:B:730:HIS:HE1	1:B:742:GLY:O	2.02	0.42
1:A:877:ASN:O	1:A:881:ILE:HG13	2.19	0.42
1:A:710:HIS:CE1	1:A:715:GLN:NE2	2.88	0.42
1:B:878:LEU:O	1:B:882:ARG:HG2	2.20	0.41
1:A:523:ILE:CG2	1:A:523:ILE:O	2.68	0.41
1:C:824:THR:CG2	1:C:859:LEU:HD13	2.50	0.41
1:A:537:ASP:OD1	1:A:539:SER:HB3	2.20	0.41
1:B:893:LYS:HD3	1:B:894:TYR:CZ	2.56	0.41
1:A:765:LEU:O	1:A:767:PRO:O	2.37	0.41
1:B:769:MET:SD	1:B:773:GLU:HG2	2.60	0.41
1:C:697:LYS:HA	1:C:697:LYS:HD2	1.81	0.41
1:C:822:TYR:HD1	1:C:864:VAL:HB	1.86	0.41
1:B:770:GLY:HA3	5:B:1015:HOH:O	2.21	0.40
1:B:867:LEU:C	1:B:869:GLU:H	2.23	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	379/423 (90%)	365 (96%)	14 (4%)	0	100	100
1	B	364/423 (86%)	351 (96%)	12 (3%)	1 (0%)	46	41
1	C	355/423 (84%)	339 (96%)	14 (4%)	2 (1%)	30	22
All	All	1098/1269 (86%)	1055 (96%)	40 (4%)	3 (0%)	46	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	808	ALA
1	C	592	ASN
1	B	518	PHE

### 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	304/336 (90%)	282 (93%)	22 (7%)	18	12
1	B	293/336 (87%)	268 (92%)	25 (8%)	13	8
1	C	286/336 (85%)	268 (94%)	18 (6%)	22	16
All	All	883/1008 (88%)	818 (93%)	65 (7%)	17	11

All (65) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	516	LEU
1	A	523	ILE
1	A	539	SER
1	A	543	GLU
1	A	574	LEU
1	A	584	ARG
1	A	594	LEU
1	A	597	LEU
1	A	623	VAL
1	A	655	ARG
1	A	656	GLU
1	A	669	HIS
1	A	692	LEU
1	A	694	GLN
1	A	765	LEU
1	A	769	MET
1	A	839	LEU
1	A	843	HIS
1	A	846	THR
1	A	862	ASN
1	A	874	GLN
1	A	878	LEU
1	B	516	LEU
1	B	519	THR
1	B	520	THR
1	B	532	GLN
1	B	535	CYS
1	B	543	GLU
1	B	568	ARG
1	B	574	LEU
1	B	584	ARG
1	B	623	VAL
1	B	625	THR
1	B	657	LEU
1	B	669	HIS
1	B	692	LEU
1	B	708	VAL
1	B	716	GLN
1	B	793	LEU
1	B	797	SER
1	B	810	LEU
1	B	839	LEU
1	B	859	LEU

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Mol	Chain	Res	Type
1	B	865	ASP
1	B	882	ARG
1	B	889	ARG
1	B	900	ARG
1	C	523	ILE
1	C	554	ARG
1	C	574	LEU
1	C	623	VAL
1	C	628	ILE
1	C	669	HIS
1	C	674	SER
1	C	692	LEU
1	C	697	LYS
1	C	706	TRP
1	C	712	ASN
1	C	734	ASP
1	C	765	LEU
1	C	810	LEU
1	C	839	LEU
1	C	859	LEU
1	C	868	SER
1	C	878	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	GLN
1	A	556	GLN
1	A	636	ASN
1	A	673	HIS
1	A	710	HIS
1	A	712	ASN
1	A	715	GLN
1	A	716	GLN
1	A	730	HIS
1	A	756	ASN
1	A	814	HIS
1	A	825	GLN
1	A	879	ASN
1	A	899	GLN
1	B	532	GLN
1	B	592	ASN

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Mol	Chain	Res	Type
1	B	636	ASN
1	B	673	HIS
1	B	710	HIS
1	B	712	ASN
1	B	715	GLN
1	B	716	GLN
1	B	730	HIS
1	B	756	ASN
1	B	825	GLN
1	B	879	ASN
1	B	899	GLN
1	C	636	ASN
1	C	673	HIS
1	C	693	GLN
1	C	710	HIS
1	C	712	ASN
1	C	715	GLN
1	C	730	HIS
1	C	756	ASN
1	C	825	GLN
1	C	874	GLN
1	C	899	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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	TSN	A	301	2	21,22,22	0.87	0	23,29,29	1.23	2 (8%)
4	TSN	B	301	2	21,22,22	0.86	1 (4%)	23,29,29	1.19	3 (13%)
4	TSN	C	301	2	21,22,22	0.75	1 (4%)	23,29,29	1.34	4 (17%)

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	TSN	A	301	2	-	2/23/23/23	0/1/1/1
4	TSN	B	301	2	-	0/23/23/23	0/1/1/1
4	TSN	C	301	2	-	0/23/23/23	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	TSN	C1-C7	2.01	1.52	1.49
4	C	301	TSN	C4-N2	2.05	1.42	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	TSN	O3-C7-C1	-2.88	116.62	120.58
4	C	301	TSN	O2-C13-C12	-2.83	117.57	123.01
4	B	301	TSN	C14-C8-C9	-2.78	108.13	110.72
4	C	301	TSN	C12-C11-C10	-2.23	122.82	126.22
4	B	301	TSN	C12-C11-C10	-2.15	122.94	126.22
4	C	301	TSN	C12-C13-N1	2.08	118.47	113.86
4	A	301	TSN	C14-C8-C9	2.34	112.89	110.72
4	C	301	TSN	C14-C8-C9	2.98	113.49	110.72
4	A	301	TSN	C12-C13-N1	3.21	120.97	113.86

There are no chirality outliers.

All (2) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	A	301	TSN	O2-C13-N1-O1
4	A	301	TSN	C12-C13-N1-O1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	TSN	2	0
4	C	301	TSN	1	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	383/423 (90%)	0.18	17 (4%) 38 39	19, 33, 52, 59	0
1	B	368/423 (86%)	0.04	18 (4%) 33 35	21, 32, 52, 60	0
1	C	359/423 (84%)	0.29	23 (6%) 23 24	25, 40, 57, 66	0
All	All	1110/1269 (87%)	0.17	58 (5%) 31 33	19, 35, 54, 66	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	796	VAL	5.9
1	C	837	LEU	4.4
1	C	867	LEU	3.9
1	C	798	ALA	3.8
1	C	797	SER	3.7
1	C	704	VAL	3.7
1	B	867	LEU	3.6
1	C	706	TRP	3.5
1	A	518	PHE	3.5
1	A	593	PRO	3.5
1	C	795	LEU	3.5
1	C	839	LEU	3.4
1	A	838	ALA	3.4
1	C	655	ARG	3.4
1	C	685	VAL	3.3
1	B	798	ALA	3.3
1	B	594	LEU	3.3
1	A	706	TRP	3.3
1	C	873	LYS	3.0
1	A	796	VAL	3.0
1	A	704	VAL	3.0
1	B	808	ALA	2.9
1	C	838	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	518	PHE	2.8
1	C	656	GLU	2.8
1	A	837	LEU	2.8
1	B	706	TRP	2.6
1	A	661	PHE	2.6
1	A	798	ALA	2.6
1	A	596	ARG	2.6
1	C	648	LEU	2.6
1	B	823	MET	2.5
1	C	661	PHE	2.5
1	B	838	ALA	2.5
1	B	592	ASN	2.5
1	A	617	PRO	2.4
1	C	841	GLY	2.4
1	B	595	SER	2.4
1	C	664	VAL	2.3
1	C	705	ASP	2.3
1	A	592	ASN	2.3
1	B	539	SER	2.3
1	A	863	ARG	2.2
1	B	584	ARG	2.2
1	B	729	LEU	2.2
1	C	694	GLN	2.2
1	C	808	ALA	2.2
1	A	594	LEU	2.2
1	B	839	LEU	2.2
1	C	654	SER	2.2
1	A	839	LEU	2.1
1	B	865	ASP	2.1
1	A	795	LEU	2.1
1	B	820	PHE	2.1
1	A	766	ASP	2.1
1	B	583	GLU	2.0
1	C	562	SER	2.0
1	B	517	PRO	2.0

## 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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	TSN	A	301	22/22	0.88	0.21	2.35	34,62,70,71	0
3	K	B	202	1/1	0.99	0.13	1.93	32,32,32,32	0
4	TSN	C	301	22/22	0.83	0.23	1.75	45,62,71,71	0
4	TSN	B	301	22/22	0.81	0.19	1.03	43,61,71,73	0
3	K	A	202	1/1	0.99	0.07	-1.12	36,36,36,36	0
2	ZN	A	102	1/1	0.99	0.05	-1.28	39,39,39,39	0
3	K	C	202	1/1	0.96	0.07	-1.33	40,40,40,40	0
2	ZN	B	102	1/1	0.98	0.05	-1.38	42,42,42,42	0
2	ZN	A	101	1/1	0.99	0.09	-1.39	29,29,29,29	0
2	ZN	C	102	1/1	0.99	0.05	-1.69	47,47,47,47	0
3	K	B	201	1/1	0.98	0.06	-2.05	30,30,30,30	0
3	K	A	201	1/1	0.99	0.04	-2.35	28,28,28,28	0
3	K	C	201	1/1	0.99	0.03	-2.74	33,33,33,33	0
2	ZN	C	101	1/1	0.99	0.05	-3.33	35,35,35,35	0
2	ZN	B	101	1/1	0.97	0.06	-3.83	34,34,34,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.