



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 07:15 AM GMT

PDB ID : 3C0Y  
Title : Crystal structure of catalytic domain of human histone deacetylase HDAC7  
Authors : Min, J.R.; Schuetz, A.; Allali-Hassani, A.; Loppnau, P.; Kwiatkowski, N.P.; Mazitschek, R.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Vedadi, M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)  
Deposited on : 2008-01-21  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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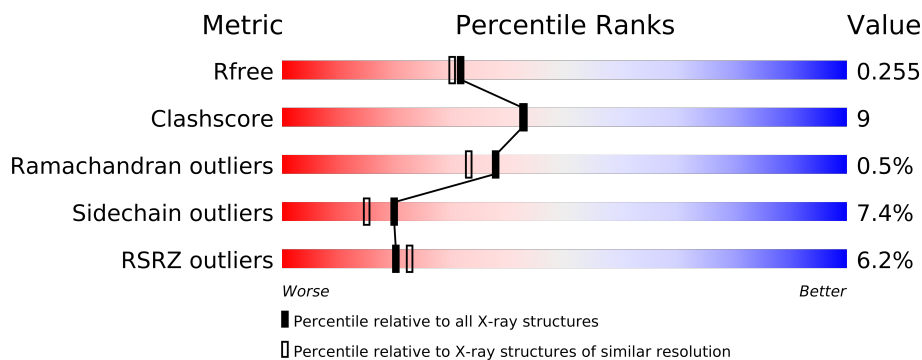
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	423	
1	B	423	
1	C	423	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8791 atoms, of which 0 are hydrogen and 0 are deuterium.

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	386	Total	C	N	O	S	0	0	0
			2925	1835	527	543	20			
1	B	367	Total	C	N	O	S	0	0	0
			2786	1745	505	517	19			
1	C	358	Total	C	N	O	S	0	0	0
			2718	1698	493	509	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 water.

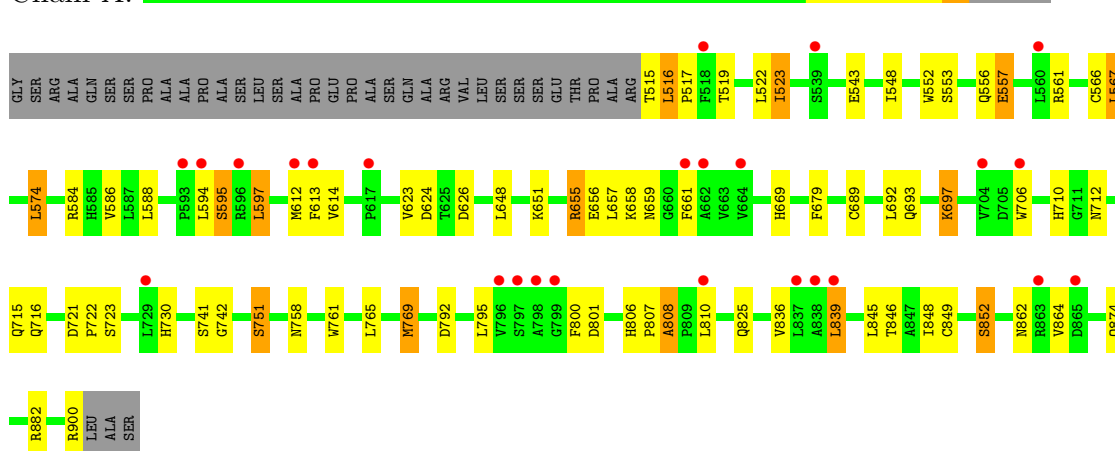
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	129	Total	O	0	0
			129	129		
4	C	99	Total	O	0	0
			99	99		

### 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.

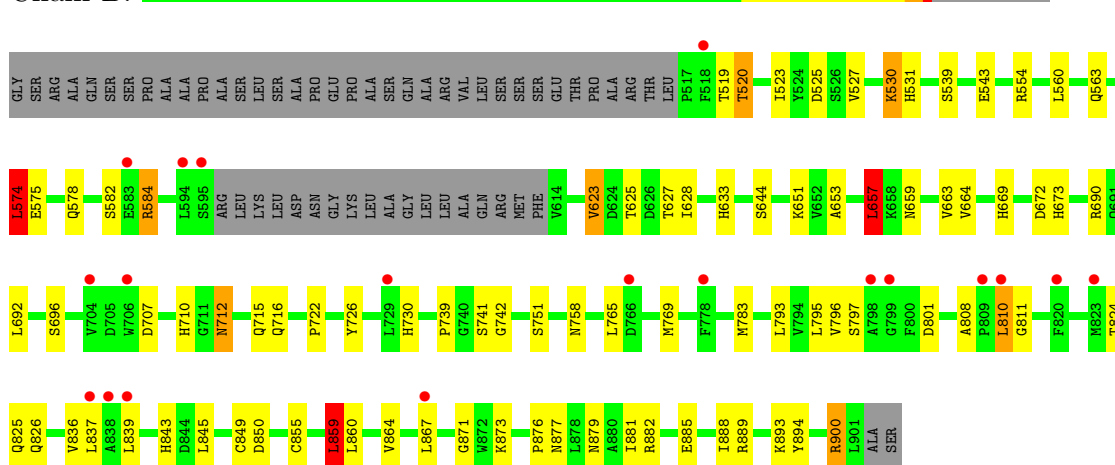
#### • Molecule 1: Histone deacetylase 7a

Chain A:



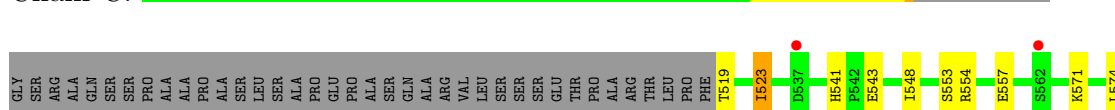
#### • Molecule 1: Histone deacetylase 7a

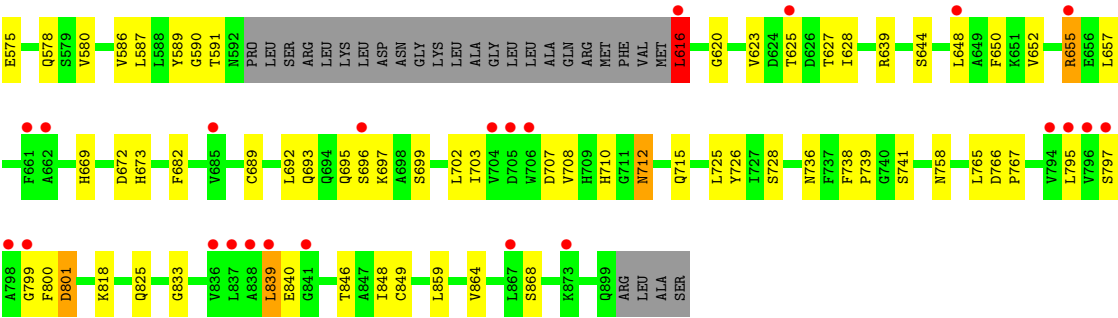
Chain B:



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

Chain C:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.75Å 81.75Å 148.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.44 – 2.10 34.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (34.44-2.10) 98.1 (34.44-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.264 0.200 , 0.255	Depositor DCC
$R_{free}$ test set	3222 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.1	EDS
Estimated twinning fraction	0.008 for -h,-k,l 0.035 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 63654 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: 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	0.90	1/2995 (0.0%)	0.91	6/4063 (0.1%)
1	B	0.90	3/2854 (0.1%)	0.92	6/3871 (0.2%)
1	C	0.76	0/2783	0.78	1/3775 (0.0%)
All	All	0.86	4/8632 (0.0%)	0.87	13/11709 (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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	855	CYS	CB-SG	-6.00	1.72	1.82
1	A	716	GLN	CB-CG	5.53	1.67	1.52
1	B	726	TYR	CD2-CE2	5.18	1.47	1.39
1	B	663	VAL	CA-CB	5.14	1.65	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	690	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	769	MET	CG-SD-CE	-6.60	89.64	100.20
1	A	516	LEU	CA-CB-CG	6.36	129.93	115.30
1	B	657	LEU	CA-CB-CG	6.29	129.77	115.30
1	B	707	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	792	ASP	CB-CG-OD2	6.14	123.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	ASP	CB-CG-OD1	5.61	123.34	118.30
1	B	574	LEU	CB-CG-CD1	5.59	120.50	111.00
1	B	859	LEU	CA-CB-CG	5.51	127.98	115.30
1	B	657	LEU	CB-CG-CD1	5.50	120.34	111.00
1	A	801	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	616	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	588	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	612	MET	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2925	0	2823	55	0
1	B	2786	0	2678	51	0
1	C	2718	0	2601	43	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	0	0
4	A	122	0	0	7	0
4	B	129	0	0	9	0
4	C	99	0	0	6	0
All	All	8791	0	8102	147	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (147) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:769:MET:HE3	4:B:329:HOH:O	1.63	0.98
1:B:575:GLU:HG3	4:B:65:HOH:O	1.70	0.91
1:B:769:MET:CE	4:B:329:HOH:O	2.17	0.91
1:A:595:SER:HB3	1:A:597:LEU:HB2	1.55	0.89
1:A:825:GLN:HE22	1:A:864:VAL:H	1.22	0.86
1:A:825:GLN:NE2	1:A:864:VAL:H	1.72	0.86
1:A:519:THR:O	1:A:658:LYS:N	2.10	0.83
1:A:715:GLN:HE22	1:A:758:ASN:HD21	1.27	0.82
1:C:825:GLN:HE22	1:C:864:VAL:H	1.23	0.82
1:B:520:THR:HB	1:B:659:ASN:OD1	1.80	0.81
1:B:525:ASP:OD2	1:B:527:VAL:HG23	1.80	0.81
1:A:810:LEU:HB2	4:A:333:HOH:O	1.81	0.79
1:B:825:GLN:HE22	1:B:864:VAL:H	1.31	0.76
1:C:586:VAL:O	1:C:590:GLY:HA3	1.89	0.72
1:A:710:HIS:HD2	1:A:741:SER:OG	1.72	0.71
1:A:658:LYS:HE2	4:A:316:HOH:O	1.90	0.71
1:C:825:GLN:NE2	1:C:864:VAL:H	1.87	0.70
1:B:715:GLN:HE22	1:B:758:ASN:HD21	1.39	0.70
1:A:655:ARG:HG2	4:C:54:HOH:O	1.92	0.69
1:C:833:GLY:O	4:C:315:HOH:O	2.10	0.68
1:B:810:LEU:HG	1:B:843:HIS:NE2	2.10	0.66
1:A:846:THR:HG23	4:A:201:HOH:O	1.95	0.66
1:C:726:TYR:CZ	1:C:728:SER:HB2	2.30	0.65
1:B:520:THR:HG23	1:B:860:LEU:HD23	1.78	0.65
1:A:595:SER:CB	1:A:597:LEU:HB2	2.26	0.64
1:A:658:LYS:HE3	1:A:659:ASN:HD21	1.62	0.64
1:C:715:GLN:HE22	1:C:758:ASN:HD21	1.47	0.62
1:C:702:LEU:HD13	1:C:725:LEU:HD23	1.81	0.62
1:B:539:SER:HB2	4:B:117:HOH:O	1.99	0.62
1:B:845:LEU:O	1:B:849:CYS:SG	2.58	0.62
1:A:656:GLU:HB2	4:C:123:HOH:O	1.99	0.62
1:A:595:SER:C	1:A:597:LEU:H	2.04	0.60
1:B:672:ASP:HB2	1:B:716:GLN:OE1	2.00	0.60
1:A:656:GLU:O	1:A:656:GLU:HG2	2.01	0.59
1:C:616:LEU:HB2	1:C:620:GLY:O	2.02	0.59
1:C:712:ASN:H	1:C:712:ASN:HD22	1.50	0.59
1:B:876:PRO:HG2	1:B:881:ILE:HD11	1.84	0.58
1:C:586:VAL:O	1:C:590:GLY:CA	2.51	0.58
1:A:721:ASP:OD1	1:A:723:SER:OG	2.18	0.58
1:B:889:ARG:NH1	4:B:50:HOH:O	2.36	0.57
4:A:251:HOH:O	1:C:591:THR:HG21	2.04	0.57
1:B:796:VAL:CG2	1:B:837:LEU:HD22	2.35	0.57
1:C:571:LYS:HB3	1:C:639:ARG:HH21	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:867:LEU:HA	4:B:93:HOH:O	2.05	0.56
1:C:818:LYS:NZ	1:C:868:SER:OG	2.39	0.56
1:A:810:LEU:HB3	4:A:290:HOH:O	2.06	0.55
1:A:651:LYS:CB	1:A:657:LEU:HD12	2.37	0.54
1:B:710:HIS:HD2	1:B:741:SER:OG	1.91	0.54
1:A:517:PRO:HG2	1:C:587:LEU:HD11	1.89	0.54
1:B:554:ARG:NH2	1:B:850:ASP:OD1	2.31	0.54
1:A:651:LYS:HD2	1:A:657:LEU:HD11	1.90	0.54
1:B:523:ILE:HG21	1:B:644:SER:HB3	1.90	0.53
1:A:761:TRP:CD2	1:A:769:MET:HE1	2.44	0.53
1:A:697:LYS:HG2	1:B:563:GLN:O	2.09	0.53
1:C:586:VAL:O	1:C:590:GLY:N	2.42	0.52
1:B:715:GLN:NE2	1:B:758:ASN:HD21	2.07	0.52
1:C:712:ASN:H	1:C:712:ASN:ND2	2.07	0.51
1:A:523:ILE:HG13	1:A:648:LEU:HB2	1.92	0.51
1:C:623:VAL:HG22	1:C:627:THR:HB	1.91	0.51
1:B:796:VAL:HG21	1:B:837:LEU:HD22	1.91	0.51
1:C:541:HIS:CE1	1:C:628:ILE:HD11	2.46	0.50
1:C:655:ARG:HB2	4:C:297:HOH:O	2.11	0.50
1:B:712:ASN:H	1:B:712:ASN:HD22	1.60	0.50
1:C:589:TYR:HB2	1:C:682:PHE:CZ	2.46	0.50
1:C:554:ARG:HE	1:C:849:CYS:HB3	1.77	0.50
1:A:722:PRO:HD3	1:A:751:SER:HB3	1.94	0.50
1:A:651:LYS:HD2	1:A:657:LEU:CD1	2.42	0.49
1:A:651:LYS:HB2	1:A:657:LEU:HD12	1.95	0.49
1:B:825:GLN:NE2	1:B:864:VAL:H	2.06	0.48
1:A:553:SER:O	1:A:557:GLU:HG3	2.13	0.48
1:A:715:GLN:NE2	1:A:758:ASN:HD21	2.04	0.48
1:B:877:ASN:OD1	1:B:879:ASN:HB2	2.13	0.48
1:A:522:LEU:HD23	1:A:661:PHE:HB3	1.96	0.48
1:B:651:LYS:HB3	1:B:657:LEU:HD22	1.96	0.48
1:B:795:LEU:HD23	1:B:836:VAL:HB	1.96	0.47
1:B:623:VAL:HG22	1:B:627:THR:HB	1.95	0.47
1:B:765:LEU:HD11	1:B:808:ALA:HB2	1.95	0.47
1:B:722:PRO:HB3	1:B:751:SER:O	2.15	0.47
1:B:584:ARG:H	1:B:584:ARG:HD3	1.79	0.47
1:C:710:HIS:HD2	1:C:741:SER:OG	1.98	0.46
1:A:552:TRP:CE3	1:A:552:TRP:HA	2.51	0.46
1:C:801:ASP:OD1	1:C:801:ASP:N	2.49	0.46
1:C:580:VAL:O	1:C:673:HIS:HD2	1.99	0.46
1:A:761:TRP:CE3	1:A:769:MET:HE1	2.51	0.46
1:A:689:CYS:O	1:A:693:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:664:VAL:O	4:B:288:HOH:O	2.20	0.46
1:A:730:HIS:HE1	1:A:742:GLY:O	1.98	0.45
1:B:628:ILE:HD12	1:B:628:ILE:C	2.37	0.45
1:C:736:ASN:ND2	4:C:306:HOH:O	2.50	0.45
1:A:567:LEU:CD2	1:A:651:LYS:HE3	2.47	0.45
1:A:825:GLN:HE22	1:A:864:VAL:N	2.02	0.45
1:A:595:SER:HB3	1:A:597:LEU:H	1.81	0.44
1:A:548:ILE:HG22	1:A:839:LEU:HD12	1.99	0.44
1:B:765:LEU:CD1	1:B:808:ALA:HB2	2.47	0.44
1:B:582:SER:HB3	1:B:673:HIS:CE1	2.52	0.44
1:B:530:LYS:HB2	1:B:633:HIS:HB3	1.99	0.44
1:C:639:ARG:HB3	1:C:639:ARG:HE	1.62	0.44
1:C:648:LEU:O	1:C:652:VAL:HG23	2.17	0.44
1:A:595:SER:C	1:A:597:LEU:N	2.70	0.44
1:A:658:LYS:HE3	1:A:659:ASN:ND2	2.32	0.44
1:A:810:LEU:CD1	4:A:333:HOH:O	2.65	0.44
1:A:567:LEU:HD22	1:A:651:LYS:HE3	1.99	0.44
1:C:672:ASP:O	1:C:673:HIS:C	2.56	0.43
1:C:707:ASP:OD2	1:C:799:GLY:HA3	2.18	0.43
1:C:554:ARG:HA	1:C:557:GLU:OE1	2.18	0.43
1:B:824:THR:CG2	1:B:859:LEU:HD13	2.49	0.43
1:A:806:HIS:HA	1:A:807:PRO:HD3	1.72	0.43
1:C:575:GLU:HA	1:C:578:GLN:HE21	1.83	0.43
1:B:885:GLU:CD	1:B:900:ARG:HH22	2.22	0.43
1:B:871:GLY:C	1:B:873:LYS:H	2.23	0.43
1:A:795:LEU:HD23	1:A:836:VAL:HB	2.01	0.43
1:B:712:ASN:H	1:B:712:ASN:ND2	2.17	0.42
1:A:552:TRP:CZ2	1:A:561:ARG:HD3	2.54	0.42
1:A:761:TRP:CD2	1:A:769:MET:CE	3.02	0.42
1:C:695:GLN:O	1:C:696:SER:C	2.57	0.42
1:A:710:HIS:CE1	1:A:715:GLN:NE2	2.88	0.42
1:B:710:HIS:CE1	1:B:715:GLN:NE2	2.87	0.42
1:B:574:LEU:O	1:B:578:GLN:HG3	2.19	0.42
1:A:848:ILE:O	1:A:852:SER:OG	2.28	0.42
1:B:696:SER:HA	4:B:102:HOH:O	2.19	0.42
1:A:810:LEU:HD13	4:A:333:HOH:O	2.20	0.42
1:A:807:PRO:O	1:A:808:ALA:C	2.58	0.42
1:A:566:CYS:C	1:A:567:LEU:HG	2.40	0.41
1:C:523:ILE:HG21	1:C:644:SER:HB3	2.01	0.41
1:C:800:PHE:HB2	1:C:848:ILE:HG22	2.02	0.41
1:B:730:HIS:HE1	1:B:742:GLY:O	2.02	0.41
1:C:766:ASP:HA	1:C:767:PRO:C	2.40	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:845:LEU:O	1:A:849:CYS:SG	2.75	0.41
1:B:739:PRO:HG2	1:B:741:SER:OG	2.21	0.41
1:A:800:PHE:HB2	1:A:848:ILE:HG22	2.02	0.41
1:B:893:LYS:HD3	1:B:894:TYR:CZ	2.56	0.41
1:C:548:ILE:HG22	1:C:839:LEU:HD12	2.03	0.41
1:C:703:ILE:HA	1:C:795:LEU:O	2.21	0.41
1:B:530:LYS:HD3	4:B:168:HOH:O	2.21	0.41
1:C:650:PHE:CZ	1:C:695:GLN:HG3	2.56	0.41
1:A:626:ASP:HB3	1:A:679:PHE:CE1	2.56	0.41
1:B:653:ALA:HB2	1:B:793:LEU:HD13	2.02	0.41
1:C:655:ARG:HD2	4:C:260:HOH:O	2.21	0.40
1:B:560:LEU:HD23	1:B:560:LEU:HA	1.76	0.40
1:A:556:GLN:HG3	1:A:561:ARG:CZ	2.52	0.40
1:C:738:PHE:HA	1:C:739:PRO:HA	1.82	0.40
1:B:783:MET:CE	1:B:826:GLN:O	2.69	0.40
1:A:574:LEU:HG	1:A:586:VAL:HG12	2.03	0.40
1:B:885:GLU:HA	1:B:888:ILE:HD12	2.04	0.40
1:C:797:SER:HB3	1:C:840:GLU:HG3	2.04	0.40
1:C:726:TYR:CE2	1:C:728:SER:HB2	2.56	0.40
1:C:689:CYS:O	1:C:693:GLN:HG3	2.21	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	384/423 (91%)	363 (94%)	18 (5%)	3 (1%)	27	20
1	B	363/423 (86%)	344 (95%)	17 (5%)	2 (1%)	33	28
1	C	354/423 (84%)	337 (95%)	17 (5%)	0	100	100
All	All	1101/1269 (87%)	1044 (95%)	52 (5%)	5 (0%)	38	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	613	PHE
1	A	808	ALA
1	B	531	HIS
1	A	557	GLU
1	B	811	GLY

### 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	306/336 (91%)	280 (92%)	26 (8%)	15	10
1	B	292/336 (87%)	273 (94%)	19 (6%)	24	20
1	C	284/336 (84%)	264 (93%)	20 (7%)	21	17
All	All	882/1008 (88%)	817 (93%)	65 (7%)	20	15

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

Mol	Chain	Res	Type
1	A	515	THR
1	A	516	LEU
1	A	523	ILE
1	A	543	GLU
1	A	567	LEU
1	A	574	LEU
1	A	584	ARG
1	A	594	LEU
1	A	595	SER
1	A	597	LEU
1	A	614	VAL
1	A	623	VAL
1	A	655	ARG
1	A	669	HIS
1	A	692	LEU
1	A	697	LYS
1	A	706	TRP
1	A	712	ASN
1	A	751	SER

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Mol	Chain	Res	Type
1	A	765	LEU
1	A	839	LEU
1	A	852	SER
1	A	862	ASN
1	A	874	GLN
1	A	882	ARG
1	A	900	ARG
1	B	519	THR
1	B	520	THR
1	B	530	LYS
1	B	543	GLU
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	712	ASN
1	B	797	SER
1	B	801	ASP
1	B	810	LEU
1	B	839	LEU
1	B	859	LEU
1	B	882	ARG
1	B	900	ARG
1	C	519	THR
1	C	523	ILE
1	C	543	GLU
1	C	553	SER
1	C	574	LEU
1	C	616	LEU
1	C	625	THR
1	C	655	ARG
1	C	657	LEU
1	C	669	HIS
1	C	692	LEU
1	C	697	LYS
1	C	699	SER
1	C	708	VAL
1	C	712	ASN
1	C	765	LEU

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Mol	Chain	Res	Type
1	C	801	ASP
1	C	839	LEU
1	C	846	THR
1	C	859	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
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	825	GLN
1	A	879	ASN
1	A	899	GLN
1	B	532	GLN
1	B	592	ASN
1	B	636	ASN
1	B	673	HIS
1	B	693	GLN
1	B	710	HIS
1	B	712	ASN
1	B	715	GLN
1	B	720	GLN
1	B	730	HIS
1	B	756	ASN
1	B	825	GLN
1	B	879	ASN
1	B	899	GLN
1	C	549	GLN
1	C	578	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

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Mol	Chain	Res	Type
1	C	756	ASN
1	C	825	GLN
1	C	879	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 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.

## 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, 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	386/423 (91%)	0.31	25 (6%)	18 20	24, 40, 62, 71	0
1	B	367/423 (86%)	0.18	19 (5%)	26 29	25, 38, 59, 71	0
1	C	358/423 (84%)	0.50	26 (7%)	15 16	31, 48, 67, 74	0
All	All	1111/1269 (87%)	0.33	70 (6%)	20 22	24, 42, 63, 74	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	837	LEU	7.0
1	C	796	VAL	6.0
1	C	798	ALA	5.5
1	C	797	SER	4.5
1	C	838	ALA	4.2
1	A	704	VAL	3.9
1	A	596	ARG	3.9
1	C	839	LEU	3.8
1	C	704	VAL	3.8
1	A	810	LEU	3.7
1	C	706	TRP	3.7
1	C	799	GLY	3.7
1	C	795	LEU	3.5
1	A	518	PHE	3.4
1	A	613	PHE	3.4
1	B	810	LEU	3.3
1	B	518	PHE	3.3
1	B	595	SER	3.2
1	A	796	VAL	3.2
1	C	867	LEU	3.1
1	A	838	ALA	3.1
1	A	797	SER	3.1
1	C	685	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	662	ALA	3.0
1	A	706	TRP	3.0
1	C	873	LYS	2.9
1	B	798	ALA	2.9
1	C	562	SER	2.8
1	A	617	PRO	2.8
1	C	661	PHE	2.7
1	A	798	ALA	2.7
1	B	706	TRP	2.6
1	A	664	VAL	2.6
1	B	729	LEU	2.6
1	B	809	PRO	2.6
1	A	593	PRO	2.5
1	C	836	VAL	2.5
1	B	778	PHE	2.5
1	B	820	PHE	2.5
1	C	794	VAL	2.5
1	C	841	GLY	2.4
1	B	594	LEU	2.4
1	C	616	LEU	2.4
1	C	648	LEU	2.4
1	C	655	ARG	2.4
1	A	661	PHE	2.4
1	B	583	GLU	2.4
1	A	837	LEU	2.4
1	A	863	ARG	2.3
1	A	799	GLY	2.3
1	B	867	LEU	2.3
1	A	865	ASP	2.2
1	C	537	ASP	2.2
1	C	705	ASP	2.2
1	A	839	LEU	2.2
1	B	838	ALA	2.2
1	B	837	LEU	2.2
1	B	704	VAL	2.2
1	B	823	MET	2.2
1	B	839	LEU	2.2
1	A	662	ALA	2.2
1	A	560	LEU	2.2
1	A	594	LEU	2.2
1	A	539	SER	2.1
1	A	612	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	696	SER	2.1
1	B	799	GLY	2.1
1	A	729	LEU	2.1
1	C	625	THR	2.0
1	B	766	ASP	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 ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	K	B	905	1/1	0.11	0.36	46,46,46,46	0
3	K	C	905	1/1	0.13	0.33	61,61,61,61	0
2	ZN	A	401	1/1	0.12	-0.65	34,34,34,34	0
2	ZN	B	404	1/1	0.05	-1.17	49,49,49,49	0
2	ZN	A	402	1/1	0.04	-1.28	46,46,46,46	0
2	ZN	C	406	1/1	0.03	-1.64	54,54,54,54	0
3	K	A	904	1/1	0.07	-1.67	33,33,33,33	0
2	ZN	B	403	1/1	0.10	-1.70	38,38,38,38	0
3	K	B	904	1/1	0.10	-1.71	38,38,38,38	0
3	K	C	904	1/1	0.08	-1.74	46,46,46,46	0
2	ZN	C	405	1/1	0.08	-2.11	43,43,43,43	0
3	K	A	905	1/1	0.05	-2.26	43,43,43,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.