



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:33 AM UTC

PDB ID : 3C0Y / pdb_00003c0y
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

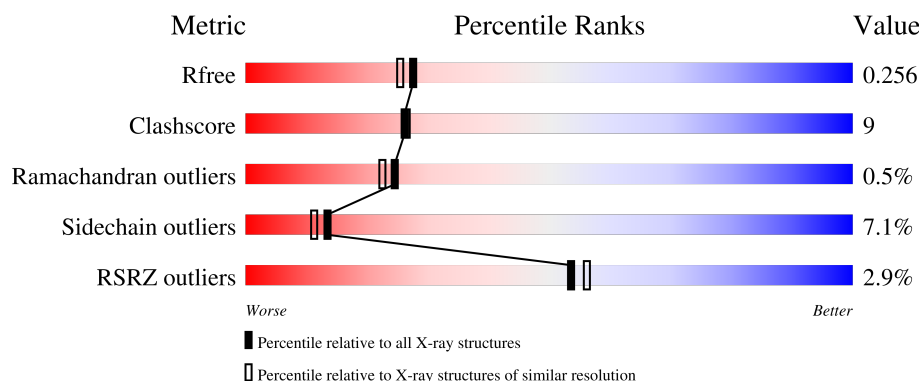
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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 $\leq 5\%$. 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	4% 73% 14% 5% 9%
1	B	423	2% 65% 18% 13%
1	C	423	2% 65% 17% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8791 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	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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

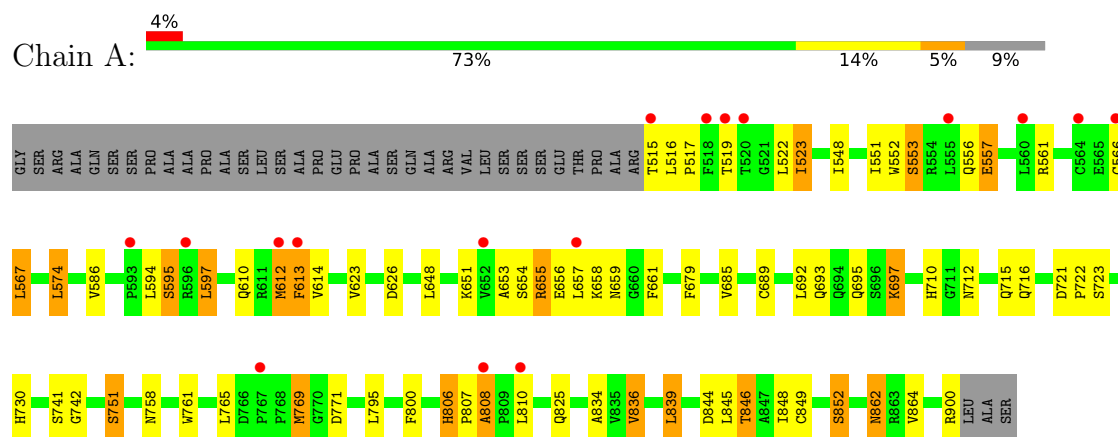
- Molecule 4 is water.

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		

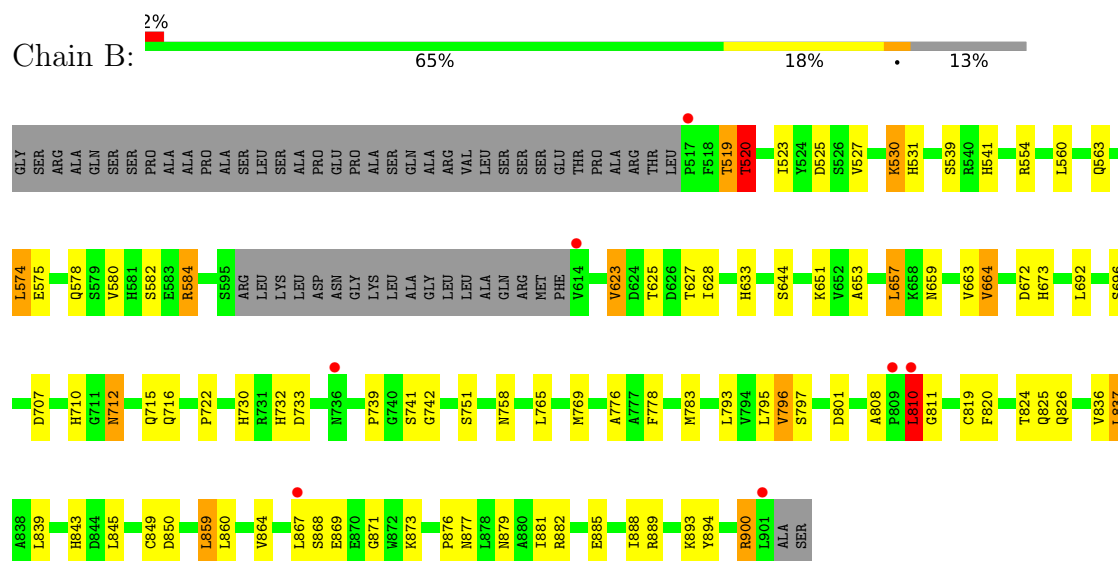
3 Residue-property plots [i](#)

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 deacetylase 7a

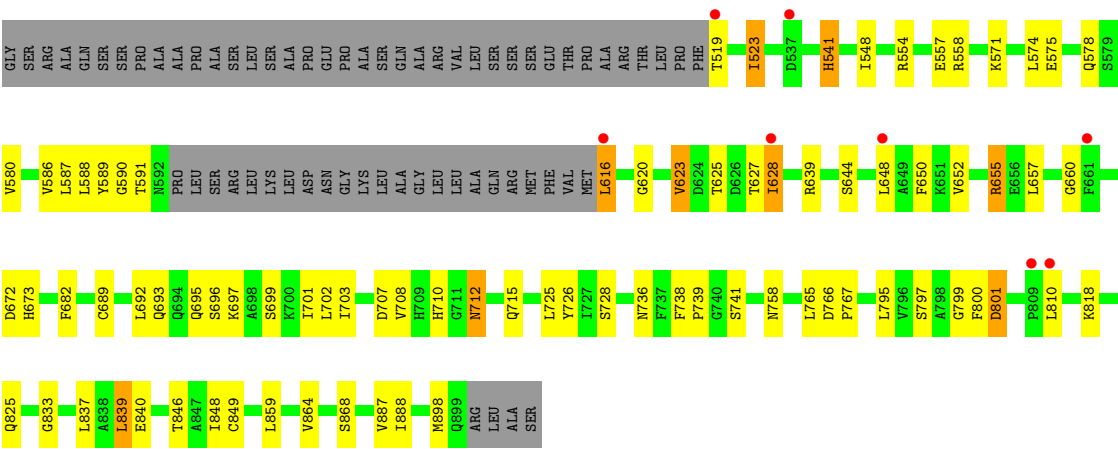


• Molecule 1: Histone deacetylase 7a



• Molecule 1: Histone deacetylase 7a





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.264 0.198 , 0.256	Depositor DCC
R_{free} test set	3222 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.035 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8791	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	1.15	5/2995 (0.2%)	1.18	10/4063 (0.2%)
1	B	1.14	5/2854 (0.2%)	1.19	8/3871 (0.2%)
1	C	0.95	1/2783 (0.0%)	1.09	4/3775 (0.1%)
All	All	1.09	11/8632 (0.1%)	1.15	22/11709 (0.2%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	663	VAL	CA-CB	8.36	1.65	1.53
1	A	846	THR	CA-CB	6.45	1.63	1.53
1	A	685	VAL	CA-CB	6.33	1.61	1.54
1	B	796	VAL	CA-CB	5.96	1.61	1.54
1	B	580	VAL	CA-CB	5.28	1.61	1.54
1	A	834	ALA	CA-C	5.24	1.59	1.52
1	B	664	VAL	CA-CB	5.21	1.62	1.55
1	C	887	VAL	CA-CB	5.09	1.60	1.54
1	B	776	ALA	CA-CB	-5.07	1.44	1.53
1	A	836	VAL	CA-CB	5.05	1.60	1.54
1	A	716	GLN	CB-CG	5.01	1.67	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	ASP	CA-C-N	-7.86	110.86	119.19
1	A	771	ASP	C-N-CA	-7.86	110.86	119.19
1	B	541	HIS	CA-C-N	7.47	127.84	119.32
1	B	541	HIS	C-N-CA	7.47	127.84	119.32
1	B	778	PHE	N-CA-C	7.29	118.87	111.07
1	B	707	ASP	N-CA-C	-6.63	100.47	110.28
1	B	868	SER	N-CA-C	-6.53	105.18	113.02
1	C	660	GLY	N-CA-C	6.46	119.34	110.56
1	A	613	PHE	N-CA-C	6.38	124.40	110.80
1	B	519	THR	CB-CA-C	-6.34	99.32	112.44
1	A	844	ASP	N-CA-C	-5.83	100.33	109.25
1	A	806	HIS	CA-C-N	5.66	125.85	120.31
1	A	806	HIS	C-N-CA	5.66	125.85	120.31
1	A	653	ALA	N-CA-C	5.51	117.29	111.28
1	B	810	LEU	N-CA-C	-5.48	106.59	113.28
1	C	810	LEU	N-CA-C	-5.48	106.64	113.38
1	C	541	HIS	CA-C-N	5.32	125.13	119.28
1	C	541	HIS	C-N-CA	5.32	125.13	119.28
1	B	520	THR	CB-CA-C	5.26	118.43	109.53
1	A	654	SER	N-CA-C	-5.25	106.38	112.89
1	A	551	ILE	N-CA-C	5.13	115.91	110.72
1	A	769	MET	CG-SD-CE	-5.12	89.64	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	612	MET	Peptide

5.2 Too-close contacts [i](#)

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	2925	0	2823	58	0
1	B	2786	0	2678	56	0
1	C	2718	0	2601	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	155	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 9.

All (155) 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:769:MET:HE1	4:B:329:HOH:O	1.56	1.06
1:B:575:GLU:HG3	4:B:65:HOH:O	1.70	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:B:769:MET:CE	4:B:329:HOH:O	2.17	0.79
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:C:888:ILE:HA	1:C:898:MET:HE3	1.76	0.66
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:A:595:SER:C	1:A:597:LEU:H	2.04	0.65
1:B:520:THR:HG23	1:B:860:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:656:GLU:HB2	4:C:123:HOH:O	1.99	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: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:HD22	1:C:712:ASN:H	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
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: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:A:848:ILE:O	1:A:852:SER:OG	2.28	0.52
1:A:523:ILE:HG13	1:A:648:LEU:HB2	1.92	0.51
1:C:712:ASN:H	1:C:712:ASN:ND2	2.07	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:B:712:ASN:H	1:B:712:ASN:HD22	1.60	0.50
1:C:655:ARG:HB2	4:C:297:HOH:O	2.11	0.50
1:C:589:TYR:HB2	1:C:682:PHE:CZ	2.46	0.50
1:A:761:TRP:CE3	1:A:769:MET:HE1	2.47	0.50
1:B:628:ILE:C	1:B:628:ILE:HD12	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:PRO:HD3	1:A:751:SER:HB3	1.94	0.50
1:C:554:ARG:HE	1:C:849:CYS:HB3	1.77	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:885:GLU:CD	1:B:900:ARG:HH22	2.22	0.48
1:A:595:SER:C	1:A:597:LEU:N	2.70	0.48
1:C:672:ASP:O	1:C:673:HIS:C	2.56	0.48
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:522:LEU:HD23	1:A:661:PHE:HB3	1.96	0.48
1:A:715:GLN:NE2	1:A:758:ASN:HD21	2.04	0.48
1:B:651:LYS:HB3	1:B:657:LEU:HD22	1.96	0.48
1:B:877:ASN:OD1	1:B:879:ASN:HB2	2.13	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:A:761:TRP:CD2	1:A:769:MET:HE2	2.50	0.47
1:B:871:GLY:C	1:B:873:LYS:H	2.23	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:HD3	1:B:584:ARG:H	1.79	0.47
1:C:695:GLN:O	1:C:696:SER:C	2.57	0.47
1:A:807:PRO:O	1:A:808:ALA:C	2.58	0.46
1:A:552:TRP:HA	1:A:552:TRP:CE3	2.51	0.46
1:C:710:HIS:HD2	1:C:741:SER:OG	1.98	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:689:CYS:O	1:A:693:GLN:HG3	2.15	0.46
1:B:664:VAL:O	4:B:288:HOH:O	2.20	0.46
1:A:566:CYS:C	1:A:567:LEU:HG	2.40	0.45
1:A:730:HIS:HE1	1:A:742:GLY:O	1.98	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:C:766:ASP:HA	1:C:767:PRO:C	2.40	0.45
1:A:825:GLN:HE22	1:A:864:VAL:N	2.02	0.45
1:A:548:ILE:HG22	1:A:839:LEU:HD12	1.99	0.44
1:A:595:SER:HB3	1:A:597:LEU:H	1.81	0.44
1:B:765:LEU:CD1	1:B:808:ALA:HB2	2.47	0.44
1:B:530:LYS:HB2	1:B:633:HIS:HB3	1.99	0.44
1:B:582:SER:HB3	1:B:673:HIS:CE1	2.52	0.44
1:B:732:HIS:O	1:B:733:ASP:C	2.60	0.44
1:C:639:ARG:HE	1:C:639:ARG:HB3	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:LEU:O	1:C:652:VAL:HG23	2.17	0.44
1:A:567:LEU:HD22	1:A:651:LYS:HE3	1.99	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: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:A:761:TRP:CD2	1:A:769:MET:CE	3.02	0.43
1:B:867:LEU:C	1:B:869:GLU:H	2.26	0.43
1:A:795:LEU:HD23	1:A:836:VAL:HB	2.01	0.43
1:A:552:TRP:CZ2	1:A:561:ARG:HD3	2.54	0.42
1:B:712:ASN:H	1:B:712:ASN:ND2	2.17	0.42
1:A:710:HIS:CE1	1:A:715:GLN:NE2	2.88	0.42
1:B:574:LEU:O	1:B:578:GLN:HG3	2.19	0.42
1:B:710:HIS:CE1	1:B:715:GLN:NE2	2.87	0.42
1:B:819:CYS:O	1:B:820:PHE:C	2.62	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:B:730:HIS:HE1	1:B:742:GLY:O	2.02	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:A:697:LYS:HG2	1:B:563:GLN:C	2.45	0.41
1:A:845:LEU:O	1:A:849:CYS:SG	2.75	0.41
1:A:862:ASN:OD1	1:A:862:ASN:C	2.63	0.41
1:A:800:PHE:HB2	1:A:848:ILE:HG22	2.02	0.41
1:B:739:PRO:HG2	1:B:741:SER:OG	2.21	0.41
1:B:783:MET:HE2	1:B:826:GLN:O	2.20	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:A:626:ASP:HB3	1:A:679:PHE:CE1	2.56	0.41
1:B:530:LYS:HD3	4:B:168:HOH:O	2.21	0.41
1:B:653:ALA:HB2	1:B:793:LEU:HD13	2.02	0.41
1:C:650:PHE:CZ	1:C:695:GLN:HG3	2.56	0.41
1:B:560:LEU:HA	1:B:560:LEU:HD23	1.76	0.40
1:C:655:ARG:HD2	4:C:260:HOH:O	2.21	0.40
1:A:556:GLN:HG3	1:A:561:ARG:CZ	2.52	0.40
1:A:574:LEU:HG	1:A:586:VAL:HG12	2.03	0.40
1:A:610:GLN:C	1:A:612:MET:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:MET:CE	1:B:826:GLN:O	2.69	0.40
1:C:738:PHE:HA	1:C:739:PRO:HA	1.82	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:689:CYS:O	1:C:693:GLN:HG3	2.21	0.40
1:C:726:TYR:CE2	1:C:728:SER:HB2	2.56	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	384/423 (91%)	363 (94%)	18 (5%)	3 (1%)	16	12
1	B	363/423 (86%)	344 (95%)	17 (5%)	2 (1%)	21	18
1	C	354/423 (84%)	337 (95%)	17 (5%)	0	100	100
All	All	1101/1269 (87%)	1044 (95%)	52 (5%)	5 (0%)	24	22

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 [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	306/336 (91%)	284 (93%)	22 (7%)	13	11
1	B	292/336 (87%)	274 (94%)	18 (6%)	16	14
1	C	284/336 (84%)	261 (92%)	23 (8%)	11	8
All	All	882/1008 (88%)	819 (93%)	63 (7%)	13	11

All (63) 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	553	SER
1	A	567	LEU
1	A	574	LEU
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	692	LEU
1	A	695	GLN
1	A	697	LYS
1	A	712	ASN
1	A	751	SER
1	A	765	LEU
1	A	839	LEU
1	A	852	SER
1	A	862	ASN
1	A	900	ARG
1	B	519	THR
1	B	520	THR
1	B	530	LYS
1	B	574	LEU
1	B	584	ARG
1	B	623	VAL
1	B	625	THR
1	B	657	LEU

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Mol	Chain	Res	Type
1	B	692	LEU
1	B	712	ASN
1	B	797	SER
1	B	801	ASP
1	B	810	LEU
1	B	837	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	558	ARG
1	C	574	LEU
1	C	588	LEU
1	C	616	LEU
1	C	623	VAL
1	C	625	THR
1	C	628	ILE
1	C	655	ARG
1	C	657	LEU
1	C	692	LEU
1	C	697	LYS
1	C	699	SER
1	C	701	ILE
1	C	708	VAL
1	C	712	ASN
1	C	765	LEU
1	C	801	ASP
1	C	837	LEU
1	C	839	LEU
1	C	846	THR
1	C	859	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	578	GLN
1	A	636	ASN
1	A	659	ASN
1	A	673	HIS
1	A	691	GLN

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Mol	Chain	Res	Type
1	A	710	HIS
1	A	712	ASN
1	A	715	GLN
1	A	716	GLN
1	A	730	HIS
1	A	736	ASN
1	A	756	ASN
1	A	825	GLN
1	A	826	GLN
1	A	879	ASN
1	B	532	GLN
1	B	556	GLN
1	B	592	ASN
1	B	636	ASN
1	B	673	HIS
1	B	691	GLN
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	556	GLN
1	C	578	GLN
1	C	673	HIS
1	C	691	GLN
1	C	693	GLN
1	C	710	HIS
1	C	712	ASN
1	C	715	GLN
1	C	716	GLN
1	C	730	HIS
1	C	732	HIS
1	C	736	ASN
1	C	825	GLN
1	C	879	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

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, 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	386/423 (91%)	0.20	17 (4%) 39 41	24, 40, 62, 71	0
1	B	367/423 (86%)	0.08	7 (1%) 66 69	25, 38, 59, 71	0
1	C	358/423 (84%)	0.37	8 (2%) 62 65	31, 48, 67, 74	0
All	All	1111/1269 (87%)	0.22	32 (2%) 53 56	24, 42, 63, 74	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	520	THR	4.2
1	B	810	LEU	3.9
1	A	810	LEU	3.7
1	B	809	PRO	3.5
1	A	566	CYS	3.4
1	B	867	LEU	3.4
1	A	518	PHE	3.4
1	A	613	PHE	3.3
1	A	593	PRO	3.1
1	A	657	LEU	2.9
1	A	560	LEU	2.7
1	B	614	VAL	2.6
1	A	515	THR	2.5
1	A	564	CYS	2.5
1	A	767	PRO	2.5
1	C	810	LEU	2.5
1	A	652	VAL	2.4
1	C	628	ILE	2.5
1	C	648	LEU	2.4
1	A	808	ALA	2.3
1	A	555	LEU	2.3
1	B	736	ASN	2.3
1	A	596	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	519	THR	2.2
1	B	901	LEU	2.2
1	C	809	PRO	2.2
1	B	517	PRO	2.2
1	C	537	ASP	2.2
1	C	616	LEU	2.2
1	A	519	THR	2.1
1	A	612	MET	2.1
1	C	661	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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
3	K	C	905	1/1	0.95	0.12	61,61,61,61	0
3	K	C	904	1/1	0.97	0.07	46,46,46,46	0
3	K	B	905	1/1	0.97	0.14	46,46,46,46	0
2	ZN	C	406	1/1	0.98	0.04	54,54,54,54	0
3	K	A	905	1/1	0.98	0.07	43,43,43,43	0
3	K	B	904	1/1	0.98	0.07	38,38,38,38	0
3	K	A	904	1/1	0.99	0.05	33,33,33,33	0
2	ZN	A	402	1/1	0.99	0.03	46,46,46,46	0
2	ZN	B	403	1/1	0.99	0.03	38,38,38,38	0
2	ZN	B	404	1/1	0.99	0.03	49,49,49,49	0
2	ZN	C	405	1/1	0.99	0.02	43,43,43,43	0
2	ZN	A	401	1/1	0.99	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.