Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:01 AM GMT

PDB ID	:	2FBM
Title	:	Acetyltransferase domain of CDY1
Authors	:	Min, J.R.; Antoshenko, T.; Hong, W.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on	:	2005-12-09
Resolution	:	2.28 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

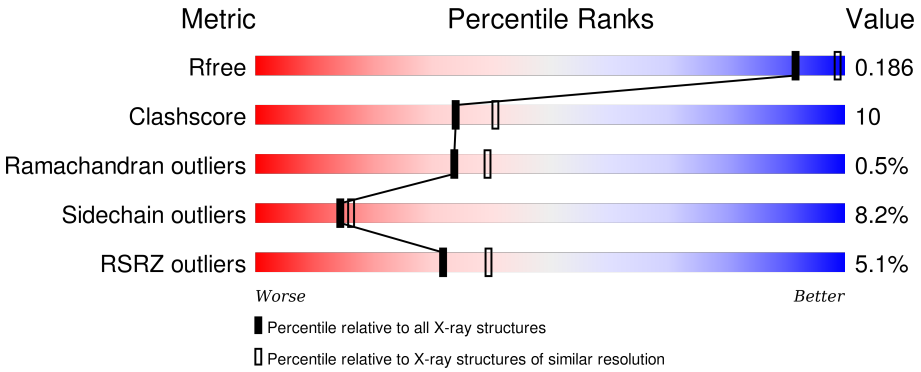
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.28 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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 >=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 <=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	291	3% 67% 16% • 14%
1	B	291	2% 62% 21% • 14%
1	C	291	8% 69% 13% • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6076 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 Y chromosome chromodomain protein 1, telomeric isoform b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1913	1221	316	362	14			
1	B	250	Total	C	N	O	S	0	0	0
			1894	1208	313	359	14			
1	C	250	Total	C	N	O	S	0	0	0
			1911	1219	319	359	14			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	MET	-	CLONING ARTIFACT	UNP Q9Y6F8
A	263	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
A	264	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
A	265	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
A	266	HIS	-	INSERTION	UNP Q9Y6F8
A	267	HIS	-	INSERTION	UNP Q9Y6F8
A	268	HIS	-	INSERTION	UNP Q9Y6F8
A	269	HIS	-	INSERTION	UNP Q9Y6F8
A	270	HIS	-	INSERTION	UNP Q9Y6F8
A	271	HIS	-	INSERTION	UNP Q9Y6F8
A	272	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
A	273	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
A	274	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
A	275	LEU	-	CLONING ARTIFACT	UNP Q9Y6F8
A	276	VAL	-	CLONING ARTIFACT	UNP Q9Y6F8
A	277	PRO	-	CLONING ARTIFACT	UNP Q9Y6F8
A	278	ARG	-	CLONING ARTIFACT	UNP Q9Y6F8
A	279	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
A	280	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
B	262	MET	-	CLONING ARTIFACT	UNP Q9Y6F8
B	263	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
B	264	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
B	265	SER	-	CLONING ARTIFACT	UNP Q9Y6F8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	266	HIS	-	INSERTION	UNP Q9Y6F8
B	267	HIS	-	INSERTION	UNP Q9Y6F8
B	268	HIS	-	INSERTION	UNP Q9Y6F8
B	269	HIS	-	INSERTION	UNP Q9Y6F8
B	270	HIS	-	INSERTION	UNP Q9Y6F8
B	271	HIS	-	INSERTION	UNP Q9Y6F8
B	272	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
B	273	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
B	274	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
B	275	LEU	-	CLONING ARTIFACT	UNP Q9Y6F8
B	276	VAL	-	CLONING ARTIFACT	UNP Q9Y6F8
B	277	PRO	-	CLONING ARTIFACT	UNP Q9Y6F8
B	278	ARG	-	CLONING ARTIFACT	UNP Q9Y6F8
B	279	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
B	280	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
C	262	MET	-	CLONING ARTIFACT	UNP Q9Y6F8
C	263	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
C	264	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
C	265	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
C	266	HIS	-	INSERTION	UNP Q9Y6F8
C	267	HIS	-	INSERTION	UNP Q9Y6F8
C	268	HIS	-	INSERTION	UNP Q9Y6F8
C	269	HIS	-	INSERTION	UNP Q9Y6F8
C	270	HIS	-	INSERTION	UNP Q9Y6F8
C	271	HIS	-	INSERTION	UNP Q9Y6F8
C	272	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
C	273	SER	-	CLONING ARTIFACT	UNP Q9Y6F8
C	274	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
C	275	LEU	-	CLONING ARTIFACT	UNP Q9Y6F8
C	276	VAL	-	CLONING ARTIFACT	UNP Q9Y6F8
C	277	PRO	-	CLONING ARTIFACT	UNP Q9Y6F8
C	278	ARG	-	CLONING ARTIFACT	UNP Q9Y6F8
C	279	GLY	-	CLONING ARTIFACT	UNP Q9Y6F8
C	280	SER	-	CLONING ARTIFACT	UNP Q9Y6F8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is water.

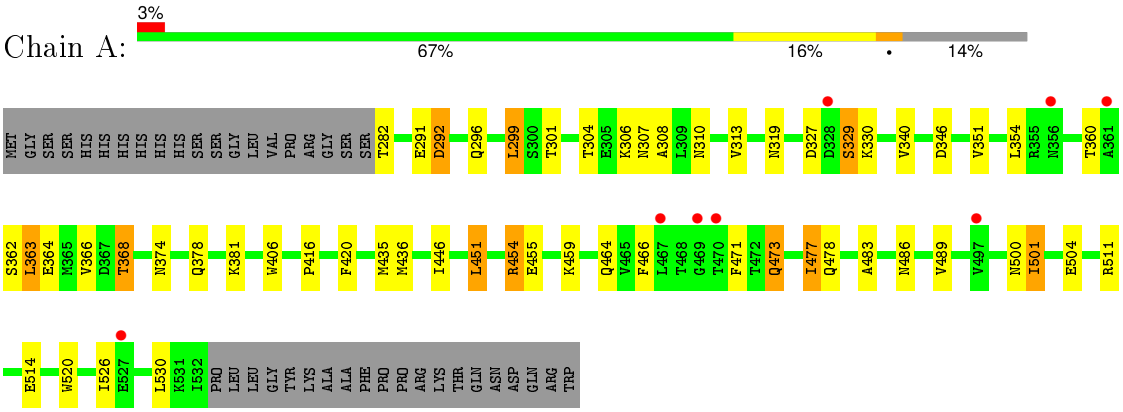
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	134	Total O 134 134	0	0
3	B	104	Total O 104 104	0	0
3	C	117	Total O 117 117	0	0

3 Residue-property plots (i)

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.

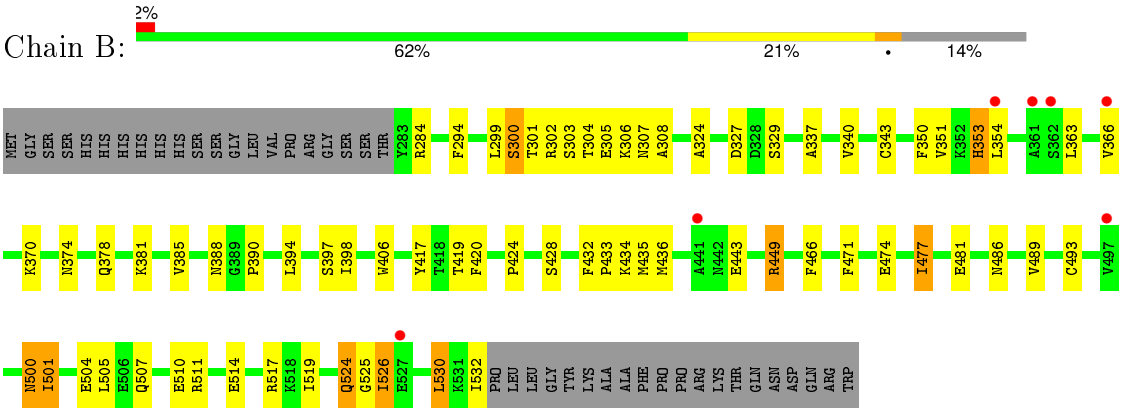
- Molecule 1: Y chromosome chromodomain protein 1, telomeric isoform b

Chain A:



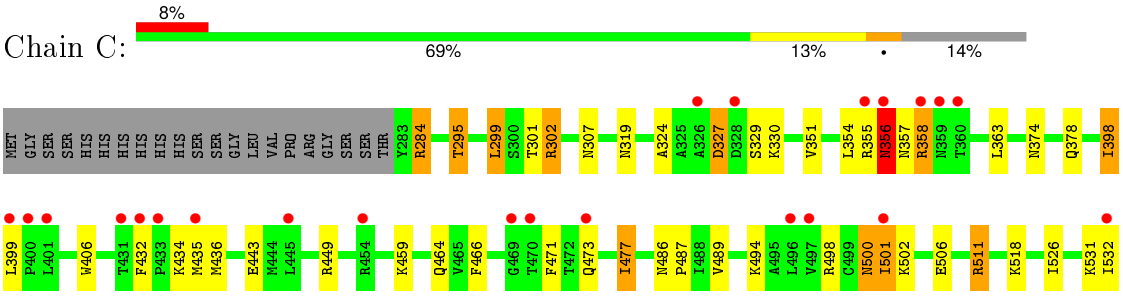
- Molecule 1: Y chromosome chromodomain protein 1, telomeric isoform b

Chain B:



- Molecule 1: Y chromosome chromodomain protein 1, telomeric isoform b

Chain C:



PRO
LEU
LEU
GLY
TYR
LYS
ALA
ALA
PHE
PRO
PRO
ARG
LYS
THR
GLN
ASN
ASP
GLN
ARG
TRP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	115.92Å 133.77Å 122.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.28 41.25 – 2.28	Depositor EDS
% Data completeness (in resolution range)	95.1 (87.71-2.28) 95.1 (41.25-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.253 0.190 , 0.186	Depositor DCC
R_{free} test set	2052 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 41375 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6076	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: CL

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	0.79	0/1943	0.78	2/2628 (0.1%)
1	B	0.71	0/1924	0.75	0/2599
1	C	0.81	2/1941 (0.1%)	0.85	3/2623 (0.1%)
All	All	0.77	2/5808 (0.0%)	0.80	5/7850 (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	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	356	ASN	CG-OD1	7.97	1.41	1.24
1	C	356	ASN	CB-CG	6.31	1.65	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	511	ARG	NE-CZ-NH2	-14.99	112.81	120.30
1	C	511	ARG	NE-CZ-NH1	11.45	126.03	120.30
1	A	511	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	511	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	363	LEU	CA-CB-CG	5.48	127.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	530	LEU	Peptide
1	C	531	LYS	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	1913	0	1937	37	0
1	B	1894	0	1915	43	0
1	C	1911	0	1942	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	134	0	0	7	0
3	B	104	0	0	5	0
3	C	117	0	0	6	0
All	All	6076	0	5794	116	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 10.

All (116) 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:500:ASN:HB2	3:B:1367:HOH:O	1.46	1.16
1:B:306:LYS:HB3	1:B:340:VAL:HG11	1.38	1.05
1:C:299:LEU:HD13	1:C:307:ASN:HB3	1.48	0.95
1:A:319:ASN:HB3	3:A:1422:HOH:O	1.68	0.94
1:C:500:ASN:H	1:C:500:ASN:HD22	1.09	0.89
1:A:464:GLN:HG2	3:A:1425:HOH:O	1.74	0.86
1:B:354:LEU:HB3	1:B:526:ILE:HD11	1.65	0.78
1:C:443:GLU:O	1:C:449:ARG:HG3	1.84	0.78
1:B:366:VAL:HG11	1:B:517:ARG:HD2	1.66	0.77
1:A:473:GLN:H	1:A:473:GLN:CD	1.90	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HD13	1:A:307:ASN:HB3	1.69	0.73
1:B:507:GLN:O	1:B:511:ARG:HG3	1.89	0.72
1:C:500:ASN:ND2	1:C:500:ASN:H	1.87	0.71
1:B:419:THR:HG23	3:B:1275:HOH:O	1.92	0.69
1:A:329:SER:O	1:A:381:LYS:HE3	1.95	0.66
1:B:406:TRP:HB3	1:B:466:PHE:CE2	2.29	0.66
1:B:306:LYS:HB3	1:B:340:VAL:CG1	2.22	0.65
1:C:327:ASP:HB3	1:C:329:SER:H	1.63	0.63
1:B:510:GLU:O	1:B:514:GLU:HG3	1.97	0.63
1:B:420:PHE:HB3	3:B:1333:HOH:O	1.99	0.63
1:C:435:MET:CE	1:C:436:MET:HE2	2.29	0.62
1:A:500:ASN:HB2	3:C:1213:HOH:O	2.01	0.61
1:A:451:LEU:HG	1:A:455:GLU:HG3	1.83	0.60
1:B:486:ASN:HB3	1:B:489:VAL:HG13	1.83	0.60
1:C:500:ASN:N	1:C:500:ASN:HD22	1.90	0.59
1:B:301:THR:HG22	3:B:1293:HOH:O	2.01	0.59
1:C:301:THR:H	1:C:307:ASN:ND2	2.01	0.58
1:C:435:MET:CE	1:C:436:MET:CE	2.82	0.58
1:B:443:GLU:O	1:B:449:ARG:HB2	2.04	0.58
1:B:504:GLU:HG3	3:B:1357:HOH:O	2.04	0.57
1:A:416:PRO:HG2	1:A:420:PHE:CZ	2.40	0.57
1:C:295:THR:HG22	1:C:329:SER:OG	2.04	0.56
1:B:394:LEU:O	1:B:398:ILE:HG13	2.06	0.56
1:A:500:ASN:CB	3:C:1213:HOH:O	2.54	0.55
1:C:356:ASN:ND2	3:C:1137:HOH:O	2.38	0.55
1:C:330:LYS:HE2	1:C:487:PRO:HG3	1.88	0.55
1:B:474:GLU:O	1:B:477:ILE:HG22	2.07	0.55
1:A:435:MET:HG3	1:A:436:MET:HG3	1.87	0.55
1:B:432:PHE:O	1:B:436:MET:HG2	2.07	0.55
1:C:299:LEU:CD1	1:C:307:ASN:HB3	2.30	0.54
1:A:381:LYS:HD3	3:A:1383:HOH:O	2.07	0.52
1:A:501:ILE:HG13	1:A:501:ILE:O	2.08	0.52
1:B:301:THR:H	1:B:307:ASN:ND2	2.07	0.52
1:C:355:ARG:HA	3:C:1216:HOH:O	2.10	0.52
1:B:300:SER:HB3	1:B:337:ALA:HB3	1.91	0.51
1:A:301:THR:H	1:A:307:ASN:ND2	2.08	0.51
1:C:532:ILE:HG12	3:C:1209:HOH:O	2.10	0.51
1:A:454:ARG:HG2	1:A:454:ARG:HH11	1.75	0.50
1:B:308:ALA:HB2	1:B:343:CYS:SG	2.52	0.50
1:C:502:LYS:HE3	1:C:506:GLU:OE2	2.11	0.50
1:B:434:LYS:HE2	1:B:501:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:TYR:CE2	1:B:424:PRO:HA	2.46	0.50
1:A:486:ASN:HD22	1:A:489:VAL:H	1.59	0.50
1:B:435:MET:CE	1:B:436:MET:CE	2.90	0.49
1:B:397:SER:HB2	1:B:428:SER:HB3	1.93	0.49
1:A:292:ASP:N	1:A:292:ASP:OD1	2.43	0.49
1:C:324:ALA:O	1:C:327:ASP:HB2	2.13	0.49
1:C:295:THR:HG22	1:C:329:SER:CB	2.43	0.49
1:B:486:ASN:HD22	1:B:489:VAL:H	1.60	0.48
1:B:327:ASP:HB3	1:B:329:SER:H	1.77	0.48
1:A:368:THR:HG21	3:A:1430:HOH:O	2.14	0.48
1:C:466:PHE:HB2	1:C:471:PHE:HD1	1.78	0.48
1:B:301:THR:HG23	1:B:304:THR:O	2.14	0.47
1:A:364:GLU:O	1:A:368:THR:HG23	2.14	0.47
1:B:294:PHE:HA	1:B:329:SER:HB2	1.97	0.47
1:B:351:VAL:HG21	1:B:530:LEU:HG	1.96	0.47
1:A:330:LYS:HD2	1:A:483:ALA:O	2.14	0.47
1:B:340:VAL:HG23	1:B:390:PRO:O	2.14	0.47
1:A:504:GLU:HG3	3:A:1361:HOH:O	2.15	0.47
1:C:511:ARG:NH2	3:C:1204:HOH:O	2.48	0.46
1:B:435:MET:HE3	1:B:436:MET:HE2	1.98	0.46
1:C:301:THR:H	1:C:307:ASN:HD22	1.62	0.46
1:C:406:TRP:HB3	1:C:466:PHE:CE2	2.50	0.45
1:C:473:GLN:O	1:C:477:ILE:HG22	2.16	0.45
1:C:299:LEU:HD13	1:C:307:ASN:CB	2.33	0.45
1:C:435:MET:HE2	1:C:436:MET:CE	2.46	0.45
1:C:432:PHE:O	1:C:436:MET:HG2	2.16	0.45
1:A:477:ILE:HD13	1:A:478:GLN:HG3	1.99	0.45
1:B:466:PHE:HB2	1:B:471:PHE:HD1	1.82	0.45
1:C:284:ARG:HE	1:C:302:ARG:HG3	1.81	0.45
1:B:374:ASN:O	1:B:378:GLN:HG2	2.17	0.45
3:A:1425:HOH:O	1:C:449:ARG:NH1	2.49	0.45
1:C:435:MET:HE2	1:C:436:MET:HE3	1.99	0.44
1:A:310:ASN:OD1	1:A:313:VAL:HG23	2.17	0.44
1:A:473:GLN:N	1:A:473:GLN:CD	2.66	0.44
1:B:432:PHE:HB2	1:B:433:PRO:HD3	2.00	0.44
1:A:514:GLU:HG2	3:A:1394:HOH:O	2.18	0.43
1:B:524:GLN:HA	1:B:524:GLN:HE21	1.84	0.43
1:C:486:ASN:HD22	1:C:489:VAL:H	1.66	0.43
1:A:374:ASN:HD21	1:A:378:GLN:HE21	1.66	0.43
1:B:514:GLU:O	1:B:517:ARG:HB2	2.19	0.43
1:A:454:ARG:NH1	1:A:454:ARG:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LEU:HD23	1:C:526:ILE:HD13	2.01	0.42
1:C:436:MET:HB2	1:C:459:LYS:HD2	2.02	0.42
1:A:406:TRP:HB3	1:A:466:PHE:CE2	2.54	0.42
1:A:327:ASP:OD2	1:A:329:SER:OG	2.30	0.42
1:B:519:ILE:O	1:B:525:GLY:HA3	2.20	0.42
1:A:351:VAL:HG21	1:A:530:LEU:HG	2.01	0.42
1:A:520:TRP:O	1:A:526:ILE:HD11	2.20	0.42
1:B:324:ALA:O	1:B:327:ASP:HB2	2.20	0.41
1:A:459:LYS:HA	1:A:459:LYS:HD3	1.89	0.41
1:B:435:MET:CE	1:B:436:MET:HE2	2.50	0.41
1:C:434:LYS:HE3	1:C:501:ILE:HD11	2.02	0.41
1:C:374:ASN:O	1:C:378:GLN:HG2	2.21	0.41
1:A:308:ALA:HB1	1:A:346:ASP:HB2	2.01	0.41
1:C:398:ILE:HD13	1:C:399:LEU:N	2.34	0.41
1:C:494:LYS:O	1:C:498:ARG:HB2	2.20	0.41
1:B:350:PHE:HD2	1:B:353:HIS:CE1	2.39	0.41
1:A:446:ILE:HD11	1:B:493:CYS:HB2	2.03	0.41
1:B:435:MET:CE	1:B:436:MET:HE3	2.50	0.41
1:A:466:PHE:HB2	1:A:471:PHE:HD1	1.85	0.40
1:B:501:ILE:HD13	1:B:505:LEU:HG	2.02	0.40
1:C:435:MET:HE1	1:C:436:MET:CE	2.51	0.40
1:A:304:THR:HB	1:A:308:ALA:HB3	2.03	0.40
1:A:362:SER:O	1:A:366:VAL:HB	2.22	0.40
1:A:301:THR:HG23	1:A:307:ASN:HD22	1.86	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	249/291 (86%)	240 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	248/291 (85%)	236 (95%)	11 (4%)	1 (0%)	39 47
1	C	248/291 (85%)	241 (97%)	4 (2%)	3 (1%)	16 15
All	All	745/873 (85%)	717 (96%)	24 (3%)	4 (0%)	34 39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	ARG
1	C	358	ARG
1	C	327	ASP
1	C	357	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/249 (84%)	192 (92%)	17 (8%)	15 17
1	B	207/249 (83%)	188 (91%)	19 (9%)	11 12
1	C	209/249 (84%)	194 (93%)	15 (7%)	18 21
All	All	625/747 (84%)	574 (92%)	51 (8%)	14 16

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	THR
1	A	291	GLU
1	A	292	ASP
1	A	296	GLN
1	A	299	LEU
1	A	306	LYS
1	A	329	SER
1	A	340	VAL
1	A	354	LEU
1	A	360	THR

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Mol	Chain	Res	Type
1	A	363	LEU
1	A	368	THR
1	A	451	LEU
1	A	454	ARG
1	A	473	GLN
1	A	477	ILE
1	A	501	ILE
1	B	299	LEU
1	B	300	SER
1	B	302	ARG
1	B	303	SER
1	B	305	GLU
1	B	353	HIS
1	B	363	LEU
1	B	370	LYS
1	B	381	LYS
1	B	385	VAL
1	B	388	ASN
1	B	449	ARG
1	B	477	ILE
1	B	481	GLU
1	B	500	ASN
1	B	501	ILE
1	B	524	GLN
1	B	526	ILE
1	B	532	ILE
1	C	284	ARG
1	C	295	THR
1	C	299	LEU
1	C	302	ARG
1	C	319	ASN
1	C	351	VAL
1	C	356	ASN
1	C	358	ARG
1	C	363	LEU
1	C	398	ILE
1	C	464	GLN
1	C	477	ILE
1	C	500	ASN
1	C	501	ILE
1	C	518	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	A	322	ASN
1	A	353	HIS
1	A	374	ASN
1	A	442	ASN
1	A	486	ASN
1	B	307	ASN
1	B	322	ASN
1	B	388	ASN
1	B	442	ASN
1	B	486	ASN
1	B	524	GLN
1	C	307	ASN
1	C	322	ASN
1	C	353	HIS
1	C	442	ASN
1	C	486	ASN
1	C	500	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	251/291 (86%)	0.15	8 (3%)	51	59	19, 27, 42, 45	0
1	B	250/291 (85%)	0.13	7 (2%)	56	65	21, 33, 57, 60	0
1	C	250/291 (85%)	0.43	23 (9%)	11	15	18, 32, 49, 53	0
All	All	751/873 (86%)	0.24	38 (5%)	32	39	18, 31, 49, 60	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	469	GLY	4.3
1	C	356	ASN	4.2
1	C	532	ILE	3.4
1	C	501	ILE	3.2
1	A	467	LEU	3.2
1	C	359	ASN	3.1
1	C	328	ASP	3.0
1	B	362	SER	2.9
1	B	497	VAL	2.9
1	A	328	ASP	2.9
1	C	400	PRO	2.8
1	C	496	LEU	2.7
1	A	469	GLY	2.7
1	C	445	LEU	2.6
1	C	470	THR	2.6
1	A	497	VAL	2.6
1	A	356	ASN	2.6
1	B	361	ALA	2.5
1	C	360	THR	2.5
1	A	361	ALA	2.5
1	B	354	LEU	2.4
1	C	497	VAL	2.4
1	A	470	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	473	GLN	2.3
1	C	454	ARG	2.3
1	B	527	GLU	2.2
1	C	433	PRO	2.2
1	A	527	GLU	2.2
1	C	431	THR	2.2
1	C	355	ARG	2.1
1	C	432	PHE	2.1
1	B	366	VAL	2.1
1	C	435	MET	2.1
1	C	326	ALA	2.0
1	C	358	ARG	2.0
1	C	401	LEU	2.0
1	B	441	ALA	2.0
1	C	399	LEU	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 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	C	1105	1/1	0.88	0.07	-	71,71,71,71	0
2	CL	B	1268	1/1	0.86	0.09	-	70,70,70,70	0
2	CL	A	1303	1/1	0.91	0.06	-	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.