



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:32 AM GMT

PDB ID : 3MCA
Title : Structure of the Dom34-Hbs1 Complex and implications for its role in No-Go decay
Authors : Chen, L.; Song, H.
Deposited on : 2010-03-28
Resolution : 2.74 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 ⓘ symbol.

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

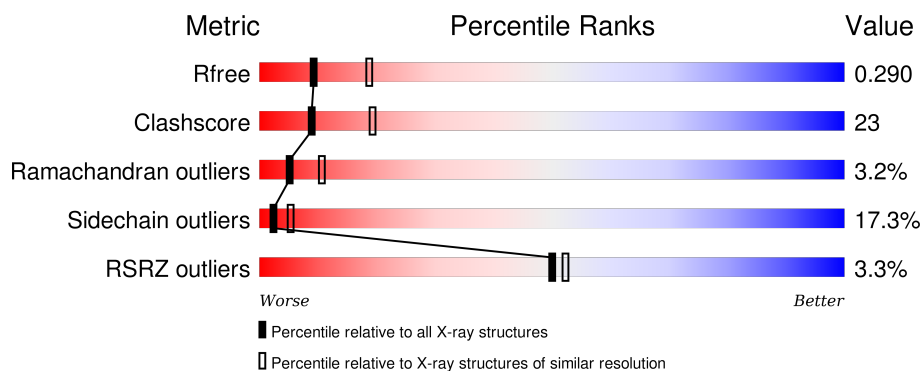
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 $\leq 5\%$. 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	592	<div> <div>5%</div> <div>38% 19% 7% 36%</div> </div>
2	B	390	<div> <div>5%</div> <div>48% 32% 7% 13%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5853 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 Elongation factor 1 alpha-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2941	1860	520	553	8			

- Molecule 2 is a protein called Protein dom34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	341	Total	C	N	O	S	0	0	0
			2744	1753	459	522	10			

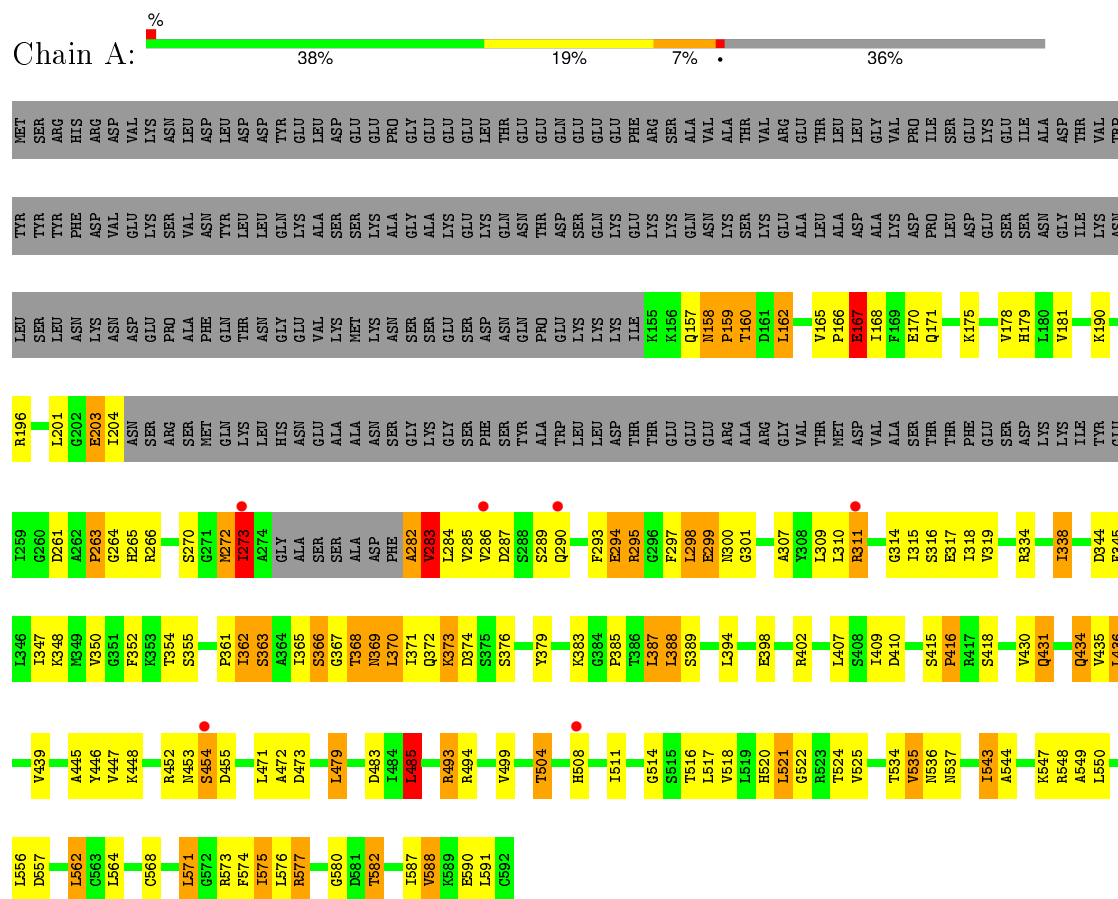
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	79	Total	O	0	0
			79	79		

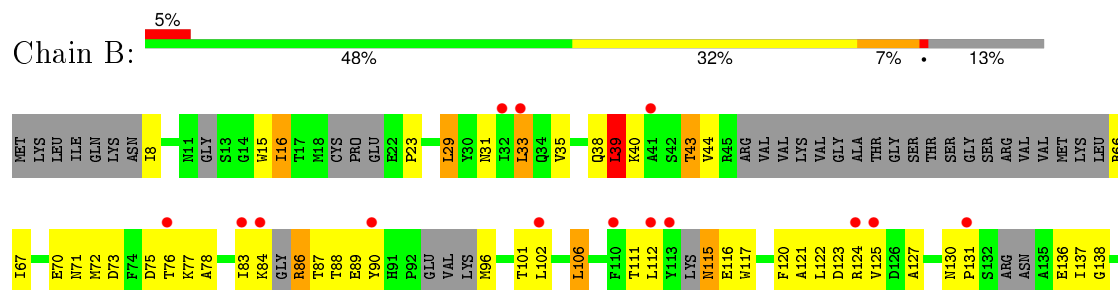
3 Residue-property plots

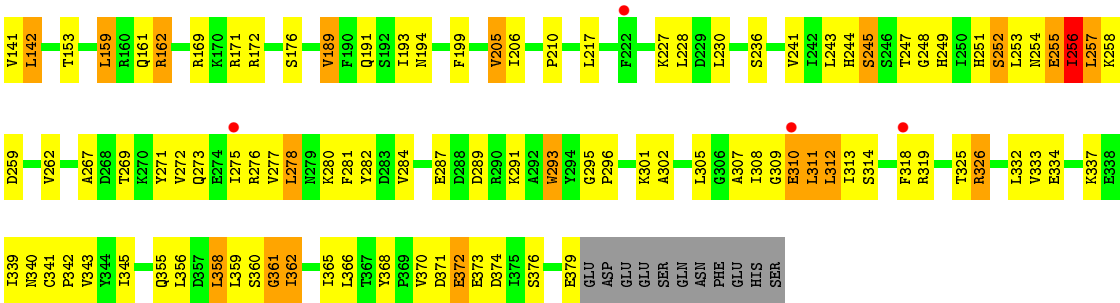
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Elongation factor 1 alpha-like protein



• Molecule 2: Protein dom34





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.74Å 113.42Å 124.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.74 83.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.74) 99.9 (83.92-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.247 , 0.286 0.248 , 0.290	Depositor DCC
R_{free} test set	1460 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 34175 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5853	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.51	0/2992	0.74	3/4055 (0.1%)
2	B	0.47	0/2793	0.69	2/3767 (0.1%)
All	All	0.49	0/5785	0.72	5/7822 (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	2
2	B	0	2
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	485	LEU	CA-CB-CG	8.44	134.70	115.30
2	B	39	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	298	LEU	CA-CB-CG	5.48	127.90	115.30
2	B	159	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	479	LEU	CA-CB-CG	5.23	127.32	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ALA	Peptide
1	A	294	GLU	Peptide
2	B	255	GLU	Peptide
2	B	256	ILE	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	2941	0	2995	143	0
2	B	2744	0	2718	126	0
3	A	89	0	0	23	0
3	B	79	0	0	11	0
All	All	5853	0	5713	265	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 23.

All (265) 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)
2:B:311:LEU:HD22	2:B:365:ILE:HB	1.17	1.16
2:B:309:GLY:H	2:B:311:LEU:HD12	1.13	1.08
1:A:504:THR:HG22	1:A:547:LYS:H	1.18	1.07
2:B:162:ARG:HH11	2:B:162:ARG:HG3	0.87	1.04
2:B:309:GLY:N	2:B:311:LEU:HD12	1.75	1.01
1:A:295:ARG:HH11	1:A:295:ARG:HG3	1.26	1.00
1:A:295:ARG:CG	1:A:295:ARG:HH11	1.75	0.99
2:B:243:LEU:HD13	2:B:256:ILE:HG21	1.45	0.98
1:A:493:ARG:HH11	1:A:493:ARG:HG2	1.30	0.96
2:B:162:ARG:HG3	2:B:162:ARG:NH1	1.66	0.96
2:B:162:ARG:CG	2:B:162:ARG:HH11	1.79	0.95
2:B:311:LEU:HD13	2:B:365:ILE:O	1.64	0.95
2:B:311:LEU:CD2	2:B:365:ILE:HB	1.96	0.94
1:A:168:ILE:HA	3:A:594:HOH:O	1.67	0.93
1:A:159:PRO:HB2	1:A:160:THR:HA	1.50	0.93
1:A:159:PRO:HB2	1:A:160:THR:CA	2.01	0.91
2:B:311:LEU:HD22	2:B:365:ILE:CB	2.01	0.91
2:B:356:LEU:O	2:B:359:LEU:O	1.88	0.90
2:B:253:LEU:O	2:B:256:ILE:O	1.91	0.89
1:A:159:PRO:CB	1:A:160:THR:HA	2.03	0.89
2:B:309:GLY:C	2:B:311:LEU:HG	1.94	0.88
2:B:161:GLN:HG3	3:B:422:HOH:O	1.72	0.88
2:B:277:VAL:HG12	2:B:313:ILE:HD11	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:GLY:HA2	2:B:360:SER:OG	1.73	0.86
2:B:310:GLU:HA	2:B:342:PRO:HD2	1.61	0.83
2:B:66:ARG:HH11	2:B:89:GLU:HG3	1.45	0.81
1:A:504:THR:HG21	1:A:544:ALA:O	1.80	0.81
1:A:298:LEU:HA	1:A:300:ASN:N	1.96	0.81
2:B:86:ARG:HA	3:B:391:HOH:O	1.80	0.81
1:A:334:ARG:O	1:A:338:ILE:HG22	1.82	0.80
1:A:289:SER:HB3	3:A:674:HOH:O	1.80	0.79
1:A:311:ARG:NH2	1:A:352:PHE:CE2	2.50	0.78
1:A:295:ARG:NH1	1:A:295:ARG:HG3	1.99	0.78
1:A:311:ARG:CZ	1:A:352:PHE:CE2	2.66	0.77
2:B:309:GLY:O	2:B:311:LEU:N	2.18	0.77
1:A:311:ARG:NH1	1:A:350:VAL:HB	1.99	0.76
1:A:167:GLU:OE1	1:A:167:GLU:O	2.03	0.76
2:B:311:LEU:HD13	2:B:365:ILE:C	2.06	0.76
2:B:121:ALA:HA	2:B:124:ARG:HH21	1.50	0.76
2:B:309:GLY:H	2:B:311:LEU:CD1	1.97	0.75
1:A:504:THR:HG22	1:A:547:LYS:N	2.00	0.75
1:A:418:SER:HA	3:A:636:HOH:O	1.85	0.75
2:B:172:ARG:HG3	3:B:470:HOH:O	1.85	0.75
2:B:257:LEU:N	2:B:257:LEU:HD22	2.01	0.75
2:B:257:LEU:H	2:B:257:LEU:HD22	1.53	0.74
2:B:309:GLY:N	2:B:311:LEU:CD1	2.51	0.73
1:A:367:GLY:HA2	3:A:593:HOH:O	1.89	0.72
2:B:251:HIS:HD2	3:B:399:HOH:O	1.72	0.72
2:B:312:LEU:HD13	2:B:314:SER:HB2	1.72	0.72
1:A:293:PHE:O	1:A:334:ARG:NH2	2.23	0.70
1:A:311:ARG:CZ	1:A:352:PHE:CD2	2.75	0.69
1:A:158:ASN:HB3	1:A:159:PRO:HD2	1.75	0.69
1:A:361:PRO:O	1:A:368:THR:HG23	1.93	0.68
1:A:298:LEU:HA	1:A:300:ASN:H	1.59	0.68
2:B:309:GLY:HA2	2:B:341:CYS:SG	2.34	0.68
2:B:319:ARG:O	2:B:319:ARG:HG3	1.93	0.68
1:A:431:GLN:H	1:A:434:GLN:NE2	1.92	0.68
2:B:361:GLY:N	3:B:434:HOH:O	2.27	0.68
1:A:383:LYS:HG3	3:A:661:HOH:O	1.94	0.67
2:B:189:VAL:HG21	2:B:217:LEU:HD21	1.77	0.67
1:A:264:GLY:HA3	3:A:622:HOH:O	1.95	0.66
1:A:181:VAL:CG1	1:A:283:VAL:HG11	2.25	0.66
1:A:493:ARG:NH1	1:A:493:ARG:HG2	1.98	0.66
2:B:40:LYS:HB3	2:B:66:ARG:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HD12	3:A:658:HOH:O	1.95	0.66
2:B:256:ILE:HG23	2:B:259:ASP:HB2	1.76	0.66
2:B:333:VAL:HG13	2:B:343:VAL:HG11	1.76	0.65
1:A:511:ILE:HB	1:A:543:ILE:HG23	1.79	0.65
2:B:307:ALA:HB1	2:B:366:LEU:HD22	1.78	0.65
1:A:286:VAL:HG22	1:A:287:ASP:N	2.12	0.64
1:A:273:ILE:CD1	3:A:675:HOH:O	2.45	0.64
2:B:311:LEU:HB3	2:B:365:ILE:H	1.62	0.64
1:A:518:VAL:HG21	2:B:247:THR:HG21	1.81	0.63
1:A:430:VAL:HA	1:A:434:GLN:HE22	1.64	0.63
2:B:121:ALA:CA	2:B:124:ARG:HH21	2.12	0.63
1:A:282:ALA:N	3:A:630:HOH:O	2.32	0.62
2:B:333:VAL:O	2:B:337:LYS:HB2	1.98	0.62
1:A:295:ARG:CG	1:A:295:ARG:NH1	2.46	0.62
1:A:314:GLY:HA3	1:A:573:ARG:HH21	1.65	0.62
1:A:159:PRO:HG3	1:A:435:VAL:HG11	1.81	0.62
2:B:271:TYR:O	2:B:275:ILE:HG12	1.99	0.62
2:B:373:GLU:HG3	3:B:409:HOH:O	1.99	0.62
2:B:257:LEU:H	2:B:257:LEU:CD2	2.12	0.61
1:A:159:PRO:CG	1:A:160:THR:HA	2.31	0.61
1:A:181:VAL:HG12	1:A:283:VAL:HG11	1.81	0.60
1:A:436:LEU:HD22	1:A:447:VAL:HG22	1.83	0.60
1:A:564:LEU:HA	1:A:588:VAL:HG22	1.84	0.60
1:A:409:ILE:HD11	1:A:485:LEU:CD1	2.30	0.60
2:B:87:THR:HG1	2:B:96:MET:N	2.00	0.60
1:A:282:ALA:N	3:A:675:HOH:O	2.34	0.59
1:A:345:PHE:O	1:A:350:VAL:HG23	2.02	0.59
2:B:360:SER:O	2:B:362:ILE:N	2.36	0.59
2:B:193:ILE:HG13	2:B:194:ASN:N	2.18	0.59
1:A:158:ASN:N	1:A:158:ASN:HD22	2.00	0.59
1:A:453:ASN:O	1:A:454:SER:O	2.21	0.59
1:A:272:MET:HA	1:A:272:MET:CE	2.33	0.58
2:B:312:LEU:CD1	2:B:314:SER:HB2	2.33	0.58
1:A:347:ILE:HD13	1:A:354:THR:HG22	1.84	0.58
1:A:493:ARG:HH11	1:A:493:ARG:CG	2.12	0.58
2:B:257:LEU:N	2:B:257:LEU:CD2	2.67	0.58
2:B:311:LEU:HB3	2:B:365:ILE:N	2.19	0.58
1:A:265:HIS:HB2	3:A:625:HOH:O	2.02	0.58
2:B:284:VAL:HG11	2:B:365:ILE:HG23	1.84	0.58
1:A:374:ASP:HB3	1:A:376:SER:OG	2.04	0.58
1:A:361:PRO:O	1:A:368:THR:CG2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PRO:HB2	1:A:160:THR:C	2.22	0.57
1:A:372:GLN:HG2	1:A:379:TYR:CE1	2.40	0.57
1:A:273:ILE:HD13	3:A:675:HOH:O	2.02	0.57
2:B:138:GLY:O	2:B:205:VAL:HA	2.04	0.57
1:A:543:ILE:CD1	1:A:549:ALA:HB2	2.34	0.57
1:A:499:VAL:HB	1:A:590:GLU:HB2	1.87	0.57
1:A:159:PRO:HG2	1:A:160:THR:HA	1.87	0.57
1:A:407:LEU:HB3	1:A:485:LEU:HD22	1.87	0.57
2:B:256:ILE:CG2	2:B:259:ASP:HB2	2.34	0.56
1:A:534:THR:HG22	1:A:550:LEU:HB3	1.87	0.56
2:B:75:ASP:O	2:B:78:ALA:HA	2.05	0.56
1:A:286:VAL:CG2	1:A:287:ASP:N	2.69	0.56
2:B:311:LEU:HD13	2:B:366:LEU:HA	1.87	0.56
1:A:286:VAL:HG13	1:A:318:ILE:HG12	1.86	0.56
1:A:434:GLN:HG2	1:A:435:VAL:N	2.20	0.56
2:B:256:ILE:HG22	2:B:259:ASP:HB3	1.88	0.56
1:A:362:ILE:HD11	1:A:387:LEU:HB2	1.86	0.56
2:B:293:TRP:HD1	2:B:302:ALA:HB2	1.71	0.56
2:B:277:VAL:HG12	2:B:313:ILE:CD1	2.32	0.55
1:A:311:ARG:NH2	1:A:352:PHE:HE2	2.02	0.55
1:A:439:VAL:HG22	1:A:494:ARG:HD3	1.87	0.55
2:B:359:LEU:O	2:B:360:SER:C	2.44	0.55
1:A:543:ILE:HD12	1:A:549:ALA:HB2	1.88	0.55
2:B:256:ILE:CG2	2:B:259:ASP:CB	2.85	0.55
2:B:255:GLU:O	2:B:258:LYS:HG2	2.07	0.55
1:A:282:ALA:HA	1:A:573:ARG:HH11	1.71	0.55
1:A:537:ASN:HB2	3:A:641:HOH:O	2.07	0.55
1:A:295:ARG:HG2	1:A:295:ARG:HH11	1.66	0.54
2:B:121:ALA:HA	2:B:124:ARG:NH2	2.19	0.54
1:A:311:ARG:NH1	1:A:350:VAL:CB	2.70	0.54
1:A:368:THR:HB	1:A:379:TYR:OH	2.07	0.54
2:B:251:HIS:CD2	3:B:399:HOH:O	2.53	0.54
1:A:286:VAL:CG1	1:A:318:ILE:HG12	2.39	0.53
2:B:249:HIS:O	2:B:252:SER:HB2	2.08	0.53
1:A:314:GLY:H	1:A:573:ARG:HE	1.57	0.52
1:A:315:ILE:H	1:A:315:ILE:HD12	1.74	0.52
2:B:368:TYR:CE1	2:B:370:VAL:HG22	2.43	0.52
1:A:273:ILE:CD1	3:A:658:HOH:O	2.55	0.52
2:B:206:ILE:HG23	2:B:243:LEU:HD12	1.90	0.52
1:A:266:ARG:NH1	1:A:394:LEU:O	2.42	0.52
2:B:66:ARG:HG2	2:B:88:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ILE:HD11	2:B:117:TRP:HE1	1.75	0.52
2:B:311:LEU:CD1	2:B:365:ILE:O	2.47	0.52
1:A:285:VAL:HG13	3:A:619:HOH:O	2.08	0.52
1:A:471:LEU:HD12	1:A:479:LEU:HD21	1.91	0.52
1:A:577:ARG:HB3	1:A:582:THR:HA	1.92	0.52
1:A:295:ARG:O	1:A:295:ARG:HD3	2.10	0.51
1:A:297:PHE:O	1:A:300:ASN:HB2	2.10	0.51
1:A:168:ILE:HD11	1:A:171:GLN:HE21	1.76	0.51
1:A:577:ARG:HE	1:A:582:THR:HG22	1.76	0.51
1:A:410:ASP:OD2	2:B:169:ARG:NH1	2.44	0.51
1:A:273:ILE:HD11	3:A:675:HOH:O	2.10	0.51
2:B:71:ASN:HB2	2:B:84:LYS:HB2	1.93	0.51
1:A:522:GLY:HA3	3:A:610:HOH:O	2.10	0.51
1:A:179:HIS:H	1:A:284:LEU:HD12	1.75	0.50
2:B:39:LEU:HB2	2:B:111:THR:O	2.11	0.50
1:A:311:ARG:NH1	1:A:350:VAL:CG1	2.74	0.50
2:B:31:ASN:ND2	2:B:319:ARG:HE	2.09	0.50
2:B:35:VAL:HG23	2:B:70:GLU:HA	1.94	0.50
2:B:310:GLU:N	2:B:311:LEU:HG	2.26	0.50
1:A:203:GLU:O	1:A:204:ILE:HB	2.12	0.50
2:B:124:ARG:HH22	2:B:326:ARG:NH2	2.10	0.50
2:B:210:PRO:HA	2:B:245:SER:O	2.12	0.50
2:B:311:LEU:HD22	2:B:365:ILE:CG2	2.42	0.49
2:B:273:GLN:O	2:B:277:VAL:HG23	2.11	0.49
2:B:254:ASN:HA	2:B:275:ILE:HD12	1.94	0.49
1:A:446:TYR:HB2	1:A:472:ALA:HB3	1.94	0.49
2:B:124:ARG:HH22	2:B:326:ARG:HH22	1.59	0.49
2:B:189:VAL:CG2	2:B:217:LEU:HD21	2.40	0.49
1:A:311:ARG:NH1	1:A:352:PHE:CD2	2.81	0.49
1:A:287:ASP:CB	1:A:319:VAL:O	2.61	0.49
1:A:311:ARG:HG3	3:A:606:HOH:O	2.13	0.49
2:B:278:LEU:O	2:B:281:PHE:HB3	2.13	0.49
2:B:29:LEU:CD2	2:B:33:LEU:HD13	2.42	0.49
1:A:289:SER:CB	3:A:674:HOH:O	2.50	0.48
1:A:285:VAL:CG1	3:A:619:HOH:O	2.62	0.48
2:B:77:LYS:N	2:B:78:ALA:HA	2.28	0.48
2:B:115:ASN:OD1	2:B:115:ASN:N	2.46	0.48
1:A:272:MET:HA	1:A:272:MET:HE3	1.95	0.48
2:B:278:LEU:HD22	2:B:282:TYR:CZ	2.48	0.48
2:B:38:GLN:HA	2:B:67:ILE:O	2.14	0.47
1:A:369:ASN:O	1:A:388:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLU:HG3	2:B:153:THR:HG23	1.96	0.47
1:A:520:HIS:NE2	1:A:577:ARG:HD3	2.29	0.47
2:B:360:SER:HB2	3:B:434:HOH:O	2.14	0.47
1:A:196:ARG:CZ	1:A:366:SER:HB3	2.45	0.47
2:B:310:GLU:HG2	2:B:342:PRO:HG2	1.96	0.47
2:B:206:ILE:CG2	2:B:243:LEU:HD12	2.44	0.47
1:A:535:VAL:HG12	1:A:536:ASN:N	2.30	0.46
1:A:170:GLU:OE1	1:A:402:ARG:NH1	2.47	0.46
2:B:256:ILE:HG22	2:B:259:ASP:CB	2.44	0.46
1:A:179:HIS:HB2	1:A:284:LEU:HG	1.97	0.46
2:B:291:LYS:O	2:B:366:LEU:N	2.49	0.46
2:B:310:GLU:O	2:B:310:GLU:CD	2.54	0.46
2:B:16:ILE:HD11	2:B:117:TRP:NE1	2.29	0.46
2:B:339:ILE:HG22	2:B:340:ASN:H	1.80	0.46
2:B:311:LEU:HD13	2:B:366:LEU:CA	2.46	0.46
1:A:168:ILE:CD1	1:A:171:GLN:HE21	2.28	0.46
1:A:409:ILE:HD12	1:A:483:ASP:HB2	1.97	0.46
2:B:43:THR:HG22	2:B:44:VAL:H	1.80	0.46
2:B:199:PHE:HB3	2:B:236:SER:OG	2.15	0.46
1:A:286:VAL:HG21	1:A:310:LEU:HD13	1.98	0.45
2:B:256:ILE:CG2	2:B:259:ASP:HB3	2.46	0.45
1:A:159:PRO:CB	1:A:435:VAL:HG21	2.47	0.45
1:A:181:VAL:O	1:A:286:VAL:HG23	2.16	0.45
1:A:370:LEU:HD22	1:A:388:LEU:HG	1.99	0.45
1:A:385:PRO:HB2	1:A:389:SER:HB3	1.99	0.45
1:A:363:SER:H	1:A:367:GLY:HA3	1.81	0.45
2:B:142:LEU:HD21	2:B:217:LEU:HD22	1.97	0.45
1:A:311:ARG:HH12	1:A:350:VAL:HB	1.79	0.45
1:A:371:ILE:HB	1:A:373:LYS:HB2	1.99	0.45
2:B:372:GLU:N	3:B:424:HOH:O	2.47	0.45
2:B:31:ASN:HB3	2:B:124:ARG:HH11	1.83	0.44
2:B:33:LEU:HD21	2:B:83:ILE:HD13	1.99	0.44
2:B:23:PRO:HA	2:B:106:LEU:HD11	1.99	0.44
1:A:301:GLY:HA3	3:A:623:HOH:O	2.18	0.44
2:B:122:LEU:HA	2:B:125:VAL:HG12	1.98	0.44
2:B:365:ILE:O	2:B:366:LEU:HD23	2.17	0.44
1:A:158:ASN:N	1:A:158:ASN:ND2	2.65	0.44
2:B:256:ILE:O	2:B:256:ILE:HD12	2.18	0.44
1:A:285:VAL:HG12	1:A:317:GLU:HB2	1.99	0.44
1:A:299:GLU:O	1:A:300:ASN:CG	2.56	0.44
2:B:121:ALA:N	2:B:124:ARG:HH21	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ARG:NH2	1:A:580:GLY:O	2.51	0.43
1:A:516:THR:OG1	2:B:355:GLN:NE2	2.50	0.43
2:B:84:LYS:HG2	2:B:101:THR:HB	2.01	0.43
1:A:372:GLN:C	1:A:374:ASP:H	2.22	0.43
2:B:244:HIS:HE1	3:B:401:HOH:O	2.02	0.43
2:B:141:VAL:HG12	2:B:248:GLY:HA2	2.01	0.42
1:A:297:PHE:HB3	3:A:680:HOH:O	2.18	0.42
1:A:445:ALA:HB1	1:A:471:LEU:HB3	2.02	0.42
1:A:571:LEU:HD12	1:A:571:LEU:HA	1.89	0.42
1:A:165:VAL:O	1:A:431:GLN:NE2	2.48	0.42
1:A:431:GLN:H	1:A:434:GLN:HE21	1.66	0.42
1:A:307:ALA:O	1:A:311:ARG:NH2	2.53	0.42
1:A:562:LEU:HD12	1:A:588:VAL:HG11	2.01	0.42
1:A:436:LEU:HD22	1:A:447:VAL:CG2	2.49	0.41
2:B:339:ILE:HG22	2:B:340:ASN:N	2.34	0.41
2:B:360:SER:C	3:B:434:HOH:O	2.56	0.41
1:A:286:VAL:HG21	1:A:310:LEU:CD1	2.50	0.41
1:A:272:MET:O	1:A:273:ILE:HG13	2.21	0.41
1:A:520:HIS:HB2	1:A:575:ILE:HG22	2.02	0.41
2:B:120:PHE:HA	2:B:123:ASP:OD2	2.20	0.41
2:B:267:ALA:HB1	2:B:276:ARG:HH21	1.86	0.41
2:B:314:SER:O	2:B:345:ILE:HA	2.19	0.41
2:B:256:ILE:HG13	2:B:256:ILE:H	1.50	0.41
2:B:31:ASN:HD22	2:B:319:ARG:HE	1.68	0.41
1:A:415:SER:CB	1:A:416:PRO:HD2	2.51	0.41
2:B:296:PRO:CA	2:B:362:ILE:HD11	2.50	0.41
1:A:514:GLY:O	2:B:358:LEU:HB3	2.21	0.41
1:A:521:LEU:CD2	1:A:574:PHE:HB3	2.50	0.41
1:A:372:GLN:O	1:A:374:ASP:N	2.54	0.41
1:A:181:VAL:HG13	1:A:283:VAL:HG11	2.01	0.41
1:A:263:PRO:CB	3:A:634:HOH:O	2.68	0.41
2:B:269:THR:OG1	2:B:272:VAL:HG23	2.21	0.41
1:A:344:ASP:O	1:A:348:LYS:HB2	2.21	0.41
2:B:318:PHE:HE2	2:B:362:ILE:HG23	1.86	0.40
1:A:190:LYS:HE2	1:A:190:LYS:HB3	1.86	0.40
2:B:130:ASN:HA	2:B:131:PRO:HD3	1.72	0.40
1:A:347:ILE:O	1:A:350:VAL:O	2.40	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	371/592 (63%)	315 (85%)	39 (10%)	17 (5%)	3	5
2	B	325/390 (83%)	297 (91%)	23 (7%)	5 (2%)	13	30
All	All	696/982 (71%)	612 (88%)	62 (9%)	22 (3%)	5	11

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	PRO
1	A	167	GLU
1	A	416	PRO
1	A	452	ARG
1	A	454	SER
2	B	127	ALA
2	B	310	GLU
2	B	361	GLY
1	A	299	GLU
1	A	366	SER
1	A	373	LYS
1	A	398	GLU
1	A	508	HIS
2	B	227	LYS
1	A	162	LEU
1	A	263	PRO
2	B	76	THR
1	A	273	ILE
1	A	283	VAL
1	A	365	ILE
1	A	535	VAL
1	A	166	PRO

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	334/523 (64%)	278 (83%)	56 (17%)	2	6
2	B	303/346 (88%)	249 (82%)	54 (18%)	2	5
All	All	637/869 (73%)	527 (83%)	110 (17%)	2	5

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	158	ASN
1	A	160	THR
1	A	162	LEU
1	A	167	GLU
1	A	175	LYS
1	A	178	VAL
1	A	201	LEU
1	A	203	GLU
1	A	261	ASP
1	A	270	SER
1	A	272	MET
1	A	273	ILE
1	A	283	VAL
1	A	290	GLN
1	A	294	GLU
1	A	295	ARG
1	A	309	LEU
1	A	311	ARG
1	A	316	SER
1	A	338	ILE
1	A	355	SER
1	A	362	ILE
1	A	363	SER
1	A	368	THR
1	A	369	ASN
1	A	370	LEU

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Mol	Chain	Res	Type
1	A	387	LEU
1	A	388	LEU
1	A	431	GLN
1	A	434	GLN
1	A	436	LEU
1	A	448	LYS
1	A	455	ASP
1	A	473	ASP
1	A	485	LEU
1	A	493	ARG
1	A	504	THR
1	A	517	LEU
1	A	521	LEU
1	A	524	THR
1	A	525	VAL
1	A	543	ILE
1	A	548	ARG
1	A	556	LEU
1	A	557	ASP
1	A	562	LEU
1	A	568	CYS
1	A	571	LEU
1	A	575	ILE
1	A	576	LEU
1	A	577	ARG
1	A	582	THR
1	A	587	ILE
1	A	588	VAL
1	A	591	LEU
2	B	8	ILE
2	B	15	TRP
2	B	16	ILE
2	B	29	LEU
2	B	33	LEU
2	B	39	LEU
2	B	43	THR
2	B	72	MET
2	B	73	ASP
2	B	86	ARG
2	B	90	TYR
2	B	102	LEU
2	B	106	LEU

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Mol	Chain	Res	Type
2	B	112	LEU
2	B	115	ASN
2	B	116	GLU
2	B	137	ILE
2	B	142	LEU
2	B	159	LEU
2	B	162	ARG
2	B	171	ARG
2	B	176	SER
2	B	189	VAL
2	B	191	GLN
2	B	205	VAL
2	B	228	LEU
2	B	230	LEU
2	B	241	VAL
2	B	245	SER
2	B	252	SER
2	B	256	ILE
2	B	257	LEU
2	B	262	VAL
2	B	278	LEU
2	B	280	LYS
2	B	287	GLU
2	B	289	ASP
2	B	293	TRP
2	B	301	LYS
2	B	305	LEU
2	B	308	ILE
2	B	311	LEU
2	B	312	LEU
2	B	325	THR
2	B	326	ARG
2	B	332	LEU
2	B	334	GLU
2	B	358	LEU
2	B	362	ILE
2	B	371	ASP
2	B	372	GLU
2	B	374	ASP
2	B	376	SER
2	B	379	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	158	ASN
1	A	171	GLN
1	A	265	HIS
1	A	369	ASN
1	A	434	GLN
1	A	453	ASN
1	A	542	HIS
2	B	31	ASN
2	B	100	HIS
2	B	115	ASN
2	B	130	ASN
2	B	251	HIS
2	B	254	ASN
2	B	355	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	377/592 (63%)	0.31	6 (1%) 74 77	40, 59, 82, 104	0
2	B	341/390 (87%)	0.44	18 (5%) 30 30	42, 69, 119, 160	0
All	All	718/982 (73%)	0.37	24 (3%) 50 52	40, 62, 109, 160	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	124	ARG	5.2
2	B	76	THR	4.6
2	B	33	LEU	3.5
2	B	112	LEU	3.3
1	A	273	ILE	3.2
2	B	90	TYR	3.1
2	B	113	TYR	2.9
2	B	84	LYS	2.8
2	B	102	LEU	2.7
2	B	310	GLU	2.7
2	B	32	ILE	2.6
2	B	41	ALA	2.5
1	A	290	GLN	2.5
2	B	110	PHE	2.5
2	B	318	PHE	2.4
1	A	311	ARG	2.3
2	B	131	PRO	2.2
1	A	508	HIS	2.2
2	B	83	ILE	2.2
2	B	275	ILE	2.2
1	A	454	SER	2.1
2	B	125	VAL	2.1
1	A	286	VAL	2.1
2	B	222	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.