



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:11 PM EDT

PDB ID : 5XFL / pdb_00005xfl
Title : Crystal structure of the force-sensing device region of alpha N-catenin
Authors : Hirano, Y.; Hakoshima, T.
Deposited on : 2017-04-10
Resolution : 2.45 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

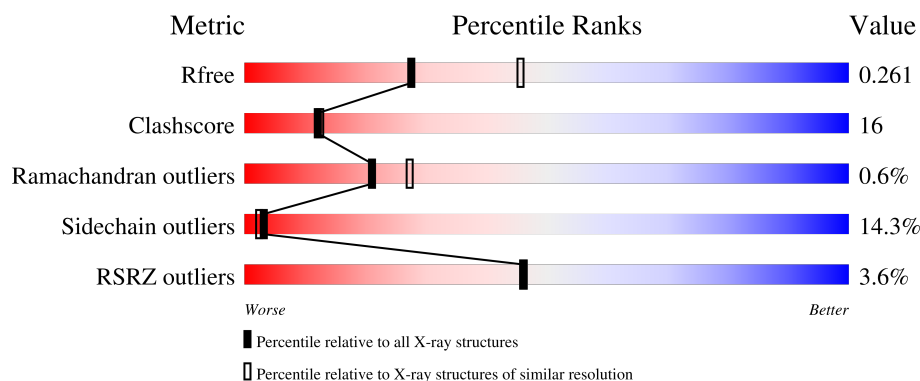
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	375	
1	B	375	
1	C	375	
1	D	375	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11346 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 Catenin alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2742	1700	482	545	15			
1	B	356	Total	C	N	O	S	0	0	0
			2747	1701	487	544	15			
1	C	359	Total	C	N	O	S	0	0	0
			2794	1731	491	557	15			
1	D	356	Total	C	N	O	S	0	0	0
			2748	1699	487	547	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	GLY	-	expression tag	UNP Q61301
A	259	PRO	-	expression tag	UNP Q61301
B	258	GLY	-	expression tag	UNP Q61301
B	259	PRO	-	expression tag	UNP Q61301
C	258	GLY	-	expression tag	UNP Q61301
C	259	PRO	-	expression tag	UNP Q61301
D	258	GLY	-	expression tag	UNP Q61301
D	259	PRO	-	expression tag	UNP Q61301

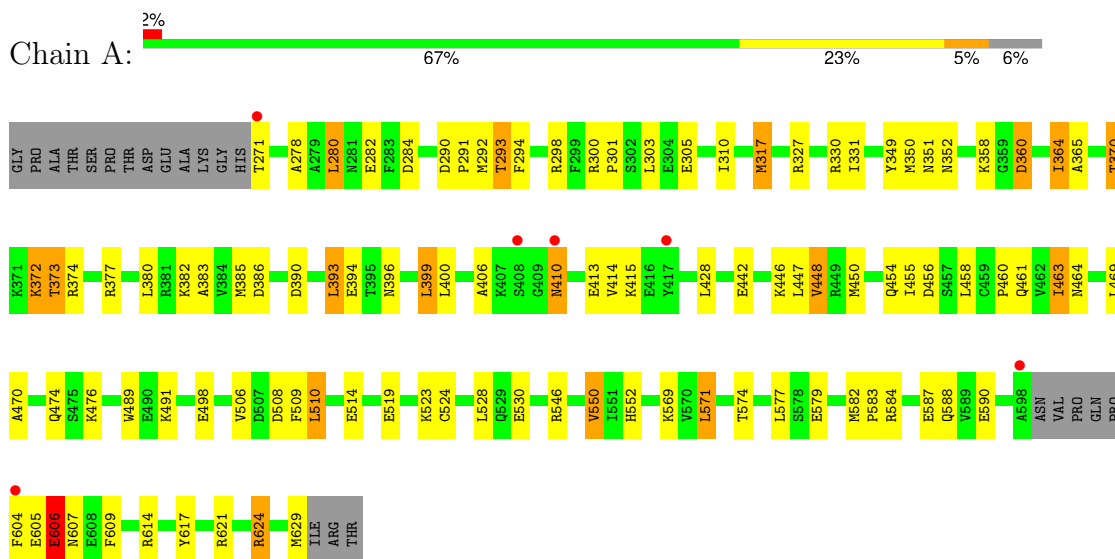
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total	O	0	0
			99	99		
2	B	105	Total	O	0	0
			105	105		
2	C	85	Total	O	0	0
			85	85		
2	D	26	Total	O	0	0
			26	26		

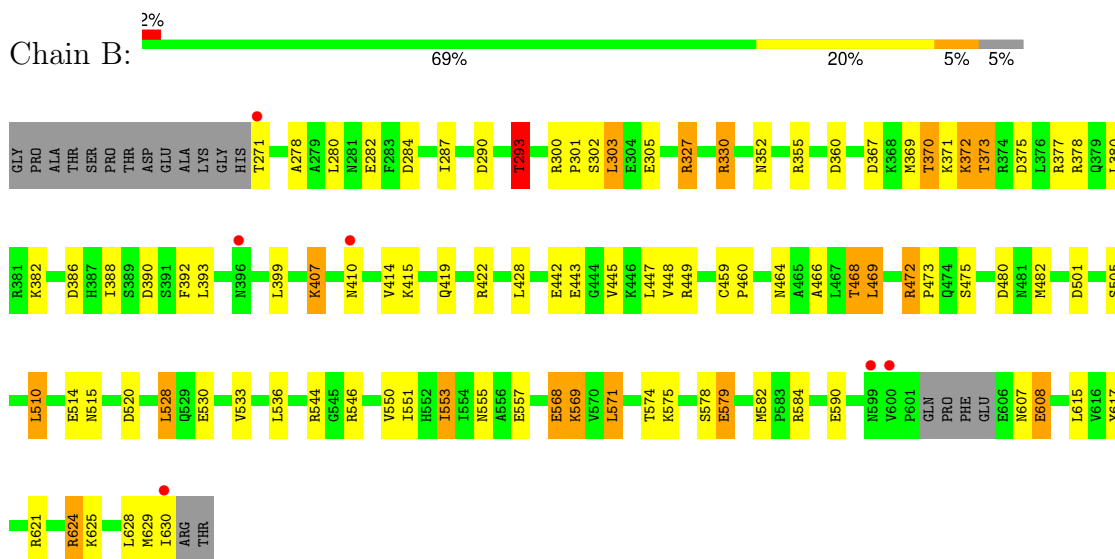
3 Residue-property plots

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.

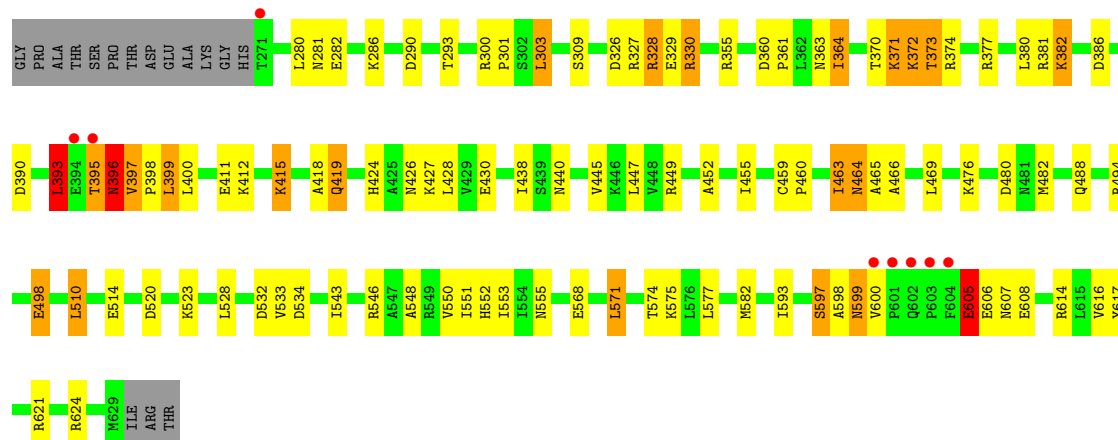
• Molecule 1: Catenin alpha-2



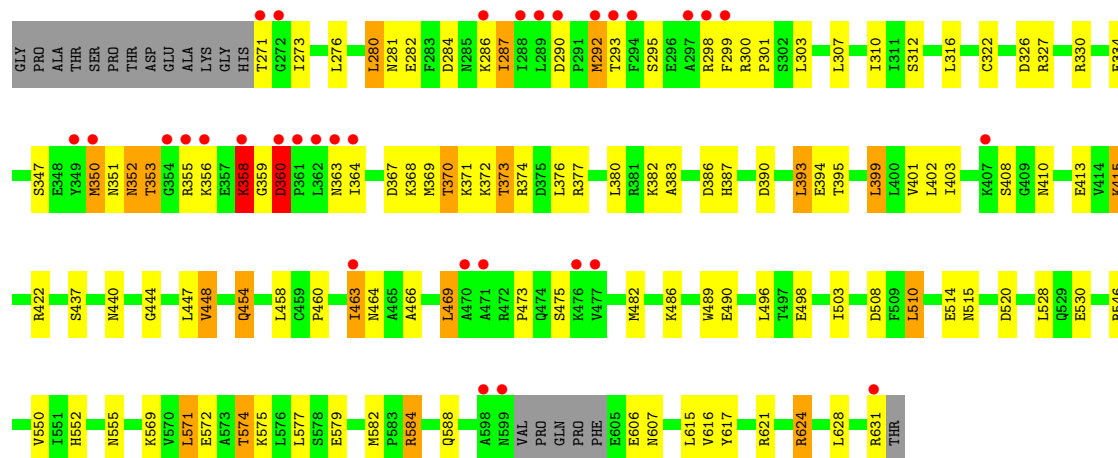
• Molecule 1: Catenin alpha-2



• Molecule 1: Catenin alpha-2



• Molecule 1: Catenin alpha-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.73Å 52.21Å 154.31Å 90.00° 95.05° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 50.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.45) 97.8 (50.00-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.267 0.220 , 0.261	Depositor DCC
R_{free} test set	3846 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11346	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.72	0/2768	0.94	3/3739 (0.1%)
1	B	0.69	0/2773	0.91	4/3747 (0.1%)
1	C	0.67	0/2823	0.87	2/3816 (0.1%)
1	D	0.56	0/2773	0.80	0/3749
All	All	0.66	0/11137	0.88	9/15051 (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
1	C	0	3
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	THR	N-CA-C	-6.18	105.78	113.38
1	A	448	VAL	N-CA-C	5.96	116.74	110.72
1	A	606	GLU	N-CA-C	-5.79	106.21	113.28
1	C	371	LYS	N-CA-C	-5.76	105.08	111.36
1	C	396	ASN	N-CA-C	5.62	122.76	110.80
1	A	550	VAL	N-CA-CB	5.08	117.45	110.54
1	B	369	MET	N-CA-C	-5.07	105.75	111.28
1	B	582	MET	CA-C-N	-5.02	113.37	118.85
1	B	582	MET	C-N-CA	-5.02	113.37	118.85

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	350	MET	Peptide
1	C	393	LEU	Peptide
1	C	395	THR	Peptide
1	C	396	ASN	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	2742	0	2731	80	0
1	B	2747	0	2739	86	0
1	C	2794	0	2796	100	0
1	D	2748	0	2734	102	0
2	A	99	0	0	4	0
2	B	105	0	0	10	0
2	C	85	0	0	1	0
2	D	26	0	0	1	0
All	All	11346	0	11000	343	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 16.

All (343) 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:466:ALA:CA	1:B:482:MET:HE1	1.66	1.25
1:B:466:ALA:HA	1:B:482:MET:CE	1.66	1.23
1:C:466:ALA:HA	1:C:482:MET:HE1	1.28	1.12
1:C:466:ALA:CA	1:C:482:MET:HE1	1.82	1.09
1:D:577:LEU:CD1	1:D:582:MET:HE3	1.81	1.09
1:B:330:ARG:HG2	1:B:330:ARG:HH11	1.12	1.08
1:C:466:ALA:HA	1:C:482:MET:CE	1.83	1.08
1:D:300:ARG:HB3	1:D:301:PRO:HD3	1.37	1.06
1:C:605:GLU:OE1	1:C:605:GLU:HA	1.48	1.06
1:C:419:GLN:HE21	1:C:419:GLN:HA	1.17	1.04
1:D:577:LEU:HD11	1:D:582:MET:HE3	1.36	1.03
1:B:330:ARG:HH11	1:B:330:ARG:CG	1.73	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:HE2	1:A:372:LYS:HA	1.39	1.00
1:C:281:ASN:HD21	1:C:440:ASN:HD21	1.06	0.99
1:C:555:ASN:HD21	1:C:574:THR:HG21	1.24	0.99
1:C:419:GLN:HA	1:C:419:GLN:NE2	1.71	0.98
1:B:327:ARG:HH22	1:B:515:ASN:ND2	1.60	0.97
1:D:358:LYS:HD2	1:D:363:ASN:HD21	1.28	0.95
1:B:466:ALA:HA	1:B:482:MET:HE1	0.97	0.95
1:A:373:THR:HG23	1:A:377:ARG:HH12	1.32	0.94
1:B:555:ASN:HD21	1:B:574:THR:HG21	1.33	0.92
1:C:605:GLU:OE1	1:C:605:GLU:CA	2.16	0.92
1:A:577:LEU:HG	1:A:582:MET:HE1	1.53	0.91
1:D:582:MET:HE1	1:D:616:VAL:HG22	1.52	0.91
1:D:370:THR:O	1:D:373:THR:HG22	1.69	0.90
1:C:281:ASN:HD21	1:C:440:ASN:ND2	1.70	0.90
1:C:372:LYS:HE2	1:C:372:LYS:HA	1.52	0.90
1:C:328:ARG:HH11	1:C:328:ARG:HG2	1.37	0.88
1:A:607:ASN:HD22	1:C:621:ARG:HH22	1.19	0.88
1:A:460:PRO:O	1:A:463:ILE:HG22	1.74	0.87
1:A:607:ASN:ND2	1:C:621:ARG:HH22	1.74	0.86
1:C:551:ILE:HD11	1:C:577:LEU:HD23	1.55	0.86
1:C:373:THR:CG2	1:C:377:ARG:HH12	1.90	0.85
1:C:466:ALA:N	1:C:482:MET:HE1	1.92	0.84
1:D:577:LEU:HD11	1:D:582:MET:CE	2.09	0.83
1:A:372:LYS:HA	1:A:372:LYS:CE	2.09	0.82
1:D:555:ASN:HD21	1:D:574:THR:HG21	1.43	0.82
1:C:494:ARG:O	1:C:498:GLU:HG2	1.81	0.80
1:D:460:PRO:O	1:D:463:ILE:HG22	1.81	0.80
1:D:466:ALA:HA	1:D:482:MET:HE1	1.63	0.80
1:A:373:THR:HG23	1:A:377:ARG:NH1	1.96	0.80
1:B:466:ALA:CB	1:B:482:MET:HE1	2.11	0.80
1:A:514:GLU:OE1	1:A:624:ARG:HD3	1.82	0.79
1:C:328:ARG:HG2	1:C:328:ARG:NH1	1.94	0.79
1:B:514:GLU:OE1	1:B:624:ARG:HD3	1.83	0.78
1:B:630:ILE:C	2:B:705:HOH:O	2.25	0.78
1:D:510:LEU:HG	1:D:624:ARG:HB2	1.66	0.78
1:C:396:ASN:O	1:C:400:LEU:HD13	1.84	0.77
1:B:284:ASP:OD1	1:B:373:THR:HG21	1.84	0.77
1:D:370:THR:HG23	1:D:374:ARG:HH22	1.50	0.77
1:C:373:THR:CG2	1:C:377:ARG:NH1	2.48	0.77
1:A:607:ASN:HD22	1:C:621:ARG:NH2	1.84	0.76
1:D:617:TYR:CE2	1:D:621:ARG:HD2	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:CG2	1:A:377:ARG:HH12	1.99	0.76
1:A:390:ASP:OD1	1:A:546:ARG:NH2	2.19	0.76
1:B:372:LYS:HE3	1:B:372:LYS:HA	1.68	0.76
1:B:551:ILE:HD13	1:B:578:SER:HB2	1.68	0.76
1:A:607:ASN:ND2	1:C:621:ARG:NH2	2.33	0.76
1:C:373:THR:HG22	1:C:377:ARG:NH1	2.01	0.76
1:C:555:ASN:ND2	1:C:574:THR:HG21	2.01	0.75
1:B:330:ARG:HG2	1:B:330:ARG:NH1	1.94	0.75
1:C:396:ASN:O	1:C:400:LEU:CD1	2.35	0.75
1:A:571:LEU:HA	1:A:574:THR:HG22	1.68	0.74
1:B:373:THR:HG23	1:B:377:ARG:HH12	1.52	0.74
1:B:382:LYS:CE	2:B:722:HOH:O	2.36	0.74
1:D:514:GLU:OE1	1:D:624:ARG:HD3	1.88	0.74
1:B:373:THR:HG23	1:B:377:ARG:NH1	2.02	0.74
1:B:617:TYR:CZ	1:B:621:ARG:HD2	2.24	0.73
1:A:291:PRO:HG3	1:A:358:LYS:HG2	1.71	0.73
1:C:328:ARG:HG3	1:C:329:GLU:N	2.04	0.73
1:B:555:ASN:ND2	1:B:574:THR:HG21	2.04	0.73
1:C:327:ARG:HD2	1:C:386:ASP:OD2	1.89	0.73
1:C:514:GLU:OE1	1:C:624:ARG:HD3	1.89	0.72
1:A:583:PRO:HG3	1:B:472:ARG:NH1	2.04	0.72
1:D:367:ASP:O	1:D:370:THR:HG22	1.90	0.71
1:D:577:LEU:CD1	1:D:582:MET:CE	2.64	0.71
1:D:466:ALA:HA	1:D:482:MET:CE	2.21	0.71
1:D:584:ARG:HH11	1:D:615:LEU:HD12	1.56	0.70
1:B:382:LYS:HE3	2:B:722:HOH:O	1.90	0.70
1:B:617:TYR:CE2	1:B:621:ARG:HD2	2.27	0.70
1:C:396:ASN:HB3	1:C:399:LEU:HB2	1.72	0.70
1:A:510:LEU:HG	1:A:624:ARG:HB2	1.73	0.70
1:D:444:GLY:O	1:D:448:VAL:HG12	1.91	0.70
1:C:373:THR:HG22	1:C:377:ARG:HH12	1.57	0.69
1:B:621:ARG:NH2	1:D:607:ASN:HD22	1.90	0.69
1:B:367:ASP:O	1:B:370:THR:HG22	1.93	0.69
1:C:555:ASN:HD21	1:C:574:THR:CG2	2.02	0.69
1:C:460:PRO:O	1:C:463:ILE:HG22	1.92	0.68
1:D:334:GLU:HA	1:D:334:GLU:OE2	1.93	0.68
1:A:577:LEU:CG	1:A:582:MET:HE1	2.23	0.68
1:D:617:TYR:CZ	1:D:621:ARG:HD2	2.28	0.68
1:A:583:PRO:HG3	1:B:472:ARG:HH12	1.59	0.67
1:D:370:THR:HG23	1:D:374:ARG:NH2	2.08	0.67
1:D:358:LYS:HD2	1:D:363:ASN:ND2	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:TYR:CE2	1:A:621:ARG:HD2	2.29	0.67
1:B:330:ARG:CG	1:B:330:ARG:NH1	2.44	0.66
1:C:390:ASP:OD1	1:C:546:ARG:NH2	2.26	0.66
1:D:382:LYS:HE3	1:D:508:ASP:OD1	1.95	0.66
1:B:607:ASN:OD1	1:D:621:ARG:NH2	2.28	0.66
1:C:571:LEU:O	1:C:574:THR:HG22	1.96	0.66
1:D:327:ARG:HH22	1:D:515:ASN:HD22	1.44	0.66
1:A:624:ARG:NH2	1:C:606:GLU:OE1	2.28	0.65
1:D:373:THR:HG23	1:D:377:ARG:HH12	1.61	0.65
1:A:552:HIS:HD2	1:B:480:ASP:OD1	1.80	0.65
1:B:327:ARG:HH22	1:B:515:ASN:HD22	1.41	0.65
1:B:372:LYS:HA	1:B:372:LYS:CE	2.27	0.65
1:B:621:ARG:HH22	1:D:607:ASN:HD22	1.45	0.65
1:C:571:LEU:HA	1:C:574:THR:HG22	1.79	0.65
1:C:551:ILE:CD1	1:C:577:LEU:HD23	2.27	0.64
1:C:617:TYR:CZ	1:C:621:ARG:HD2	2.31	0.64
1:C:326:ASP:OD2	1:C:330:ARG:HD2	1.96	0.64
1:A:284:ASP:OD1	1:A:373:THR:HG21	1.98	0.64
1:B:472:ARG:HG2	1:B:475:SER:HB2	1.78	0.64
1:B:371:LYS:NZ	1:B:375:ASP:OD2	2.27	0.64
1:C:327:ARG:HD3	1:C:382:LYS:HB3	1.80	0.64
1:B:327:ARG:HD2	1:B:386:ASP:OD2	1.98	0.64
1:A:461:GLN:HA	1:A:464:ASN:HD22	1.63	0.63
1:A:624:ARG:HH22	1:C:606:GLU:CD	2.06	0.63
1:B:621:ARG:NH2	1:D:607:ASN:ND2	2.46	0.63
1:C:463:ILE:CG2	1:C:464:ASN:N	2.61	0.63
1:D:373:THR:HG23	1:D:377:ARG:NH1	2.14	0.63
1:D:577:LEU:HD12	1:D:582:MET:HE3	1.79	0.63
1:A:577:LEU:HG	1:A:582:MET:CE	2.29	0.62
1:C:396:ASN:HA	1:C:398:PRO:HD2	1.82	0.62
1:D:454:GLN:O	1:D:458:LEU:HB2	2.00	0.62
1:D:631:ARG:HG2	1:D:631:ARG:HH11	1.65	0.62
1:D:327:ARG:HH22	1:D:515:ASN:ND2	1.97	0.62
1:A:617:TYR:CZ	1:A:621:ARG:HD2	2.35	0.61
1:B:443:GLU:CD	1:B:443:GLU:H	2.08	0.61
1:D:300:ARG:CB	1:D:301:PRO:HD3	2.23	0.61
1:D:466:ALA:CA	1:D:482:MET:HE1	2.30	0.61
1:A:330:ARG:NH2	1:C:532:ASP:OD2	2.33	0.61
1:D:300:ARG:HB3	1:D:301:PRO:CD	2.20	0.61
1:D:584:ARG:NH1	1:D:615:LEU:HD12	2.15	0.61
1:A:271:THR:HA	1:A:442:GLU:OE2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:ASP:OD1	1:D:546:ARG:NH2	2.34	0.60
1:A:280:LEU:HD13	1:A:310:ILE:HD13	1.83	0.60
1:A:327:ARG:HD2	1:A:386:ASP:OD2	2.01	0.60
1:D:582:MET:CE	1:D:616:VAL:HG22	2.28	0.60
1:A:370:THR:CG2	1:A:374:ARG:NH1	2.64	0.60
1:C:300:ARG:HB3	1:C:301:PRO:HD3	1.84	0.60
1:A:382:LYS:HE3	1:A:508:ASP:OD1	2.02	0.60
1:B:571:LEU:HA	1:B:574:THR:HG22	1.82	0.60
1:D:322:CYS:HB2	1:D:387:HIS:CD2	2.37	0.60
1:D:292:MET:HB2	1:D:356:LYS:HA	1.82	0.59
1:C:617:TYR:CE2	1:C:621:ARG:HD2	2.38	0.59
1:A:571:LEU:O	1:A:574:THR:HG22	2.02	0.59
1:B:466:ALA:HA	1:B:482:MET:HE2	1.74	0.59
1:D:293:THR:O	1:D:293:THR:HG23	2.02	0.59
1:B:327:ARG:HH22	1:B:515:ASN:HD21	1.49	0.58
1:A:278:ALA:O	1:A:282:GLU:HG2	2.04	0.58
1:C:419:GLN:HE21	1:C:419:GLN:CA	1.93	0.58
1:C:419:GLN:NE2	1:C:419:GLN:CA	2.49	0.58
1:B:621:ARG:HH22	1:D:607:ASN:ND2	2.01	0.57
1:D:295:SER:O	1:D:299:PHE:HB2	2.04	0.57
1:A:571:LEU:HD12	1:A:574:THR:HG21	1.86	0.57
1:B:419:GLN:HA	1:B:419:GLN:NE2	2.17	0.57
1:D:448:VAL:HG11	1:D:503:ILE:HD13	1.86	0.57
1:C:582:MET:N	1:C:582:MET:HE2	2.19	0.57
1:D:575:LYS:O	1:D:579:GLU:HB2	2.04	0.57
1:B:544:ARG:HD2	2:B:768:HOH:O	2.05	0.57
1:C:577:LEU:HG	1:C:582:MET:HE3	1.87	0.56
1:B:300:ARG:HB3	1:B:301:PRO:HD3	1.88	0.56
1:B:382:LYS:HE2	2:B:722:HOH:O	1.98	0.56
1:B:390:ASP:OD1	1:B:546:ARG:NH2	2.36	0.56
1:C:463:ILE:HG22	1:C:464:ASN:N	2.22	0.55
1:D:399:LEU:O	1:D:399:LEU:HD22	2.06	0.55
1:B:501:ASP:CG	1:B:553:ILE:HD11	2.31	0.55
1:D:498:GLU:OE2	1:D:552:HIS:HE1	1.89	0.55
1:A:364:ILE:HG13	1:A:365:ALA:N	2.22	0.55
1:C:582:MET:HE1	1:C:616:VAL:HG22	1.88	0.55
1:C:466:ALA:HA	1:C:482:MET:HE3	1.83	0.54
1:A:571:LEU:HA	1:A:574:THR:CG2	2.35	0.54
1:B:575:LYS:HG3	1:B:579:GLU:OE2	2.07	0.54
1:C:598:ALA:C	1:C:600:VAL:H	2.16	0.54
1:C:397:VAL:N	1:C:398:PRO:CD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:HE2	1:A:372:LYS:CA	2.15	0.53
1:D:469:LEU:HD22	1:D:473:PRO:HA	1.89	0.53
1:B:608:GLU:HG2	2:B:726:HOH:O	2.08	0.53
1:A:454:GLN:O	1:A:458:LEU:HB2	2.07	0.53
1:A:360:ASP:O	1:A:364:ILE:HG23	2.09	0.53
1:B:290:ASP:O	1:B:293:THR:HG22	2.09	0.53
1:B:555:ASN:HD21	1:B:574:THR:CG2	2.13	0.53
1:D:358:LYS:O	1:D:358:LYS:HG3	2.09	0.52
1:B:625:LYS:NZ	1:D:607:ASN:HD21	2.08	0.52
1:A:294:PHE:CD1	1:A:294:PHE:C	2.87	0.52
1:C:281:ASN:ND2	1:C:440:ASN:HD21	1.90	0.52
1:D:327:ARG:HD3	1:D:382:LYS:HB3	1.91	0.52
1:D:352:ASN:CG	1:D:352:ASN:O	2.53	0.52
1:B:520:ASP:OD2	1:B:546:ARG:NH1	2.41	0.51
1:A:372:LYS:CE	1:A:372:LYS:CA	2.82	0.51
1:C:605:GLU:OE1	1:C:605:GLU:N	2.42	0.51
1:D:383:ALA:O	1:D:386:ASP:HB2	2.10	0.51
1:A:327:ARG:HD3	1:A:382:LYS:HB3	1.93	0.51
1:B:568:GLU:OE2	1:B:568:GLU:HA	2.10	0.50
1:C:577:LEU:CD1	1:C:582:MET:HE3	2.41	0.50
1:C:330:ARG:NH1	2:C:703:HOH:O	2.44	0.50
1:C:465:ALA:C	1:C:482:MET:HE1	2.36	0.50
1:A:410:ASN:CB	1:A:413:GLU:HG3	2.42	0.50
1:D:371:LYS:O	1:D:374:ARG:HB3	2.11	0.50
1:C:360:ASP:HB2	1:C:361:PRO:HD2	1.94	0.50
1:D:359:GLY:O	1:D:360:ASP:C	2.55	0.50
1:D:282:GLU:O	1:D:286:LYS:HB2	2.11	0.50
1:D:347:SER:HA	1:D:350:MET:HE2	1.94	0.50
1:C:328:ARG:HH11	1:C:328:ARG:CG	2.14	0.49
1:D:284:ASP:OD1	1:D:373:THR:HG21	2.12	0.49
1:D:399:LEU:HD22	1:D:403:ILE:HG13	1.93	0.49
1:A:524:CYS:HB3	1:A:609:PHE:CZ	2.47	0.49
1:D:498:GLU:OE2	1:D:552:HIS:CE1	2.66	0.49
1:B:378:ARG:HD3	2:B:716:HOH:O	2.11	0.49
1:C:290:ASP:HB3	1:C:293:THR:HG23	1.95	0.49
1:B:624:ARG:NH2	1:D:606:GLU:OE1	2.45	0.49
1:D:326:ASP:OD2	1:D:330:ARG:NH1	2.45	0.49
1:A:571:LEU:CA	1:A:574:THR:HG22	2.39	0.49
1:D:327:ARG:HD2	1:D:386:ASP:OD2	2.12	0.49
1:B:278:ALA:O	1:B:282:GLU:HG2	2.12	0.48
1:B:624:ARG:HH22	1:D:606:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:LEU:HA	1:C:574:THR:CG2	2.43	0.48
1:A:385:MET:HE2	1:A:509:PHE:HA	1.94	0.48
1:D:290:ASP:CG	1:D:293:THR:HG22	2.38	0.48
1:A:300:ARG:HB3	1:A:301:PRO:HD3	1.96	0.48
1:C:396:ASN:HD21	1:C:424:HIS:CD2	2.32	0.48
1:D:355:ARG:HG2	1:D:355:ARG:HH11	1.79	0.48
1:B:510:LEU:HG	1:B:624:ARG:HB2	1.96	0.48
1:A:282:GLU:OE2	2:A:701:HOH:O	2.20	0.48
1:A:393:LEU:O	1:A:394:GLU:C	2.57	0.47
1:B:271:THR:HA	1:B:442:GLU:OE2	2.14	0.47
1:B:382:LYS:NZ	1:D:530:GLU:OE1	2.48	0.47
1:D:489:TRP:O	1:D:490:GLU:C	2.57	0.47
1:A:474:GLN:H	1:A:474:GLN:CD	2.23	0.47
1:A:552:HIS:HD2	1:B:480:ASP:CG	2.23	0.47
1:A:552:HIS:CD2	1:B:480:ASP:OD1	2.66	0.47
1:B:557:GLU:O	1:B:557:GLU:HG3	2.15	0.47
1:C:520:ASP:HB3	1:C:543:ILE:HG13	1.97	0.47
1:C:548:ALA:O	1:C:552:HIS:CD2	2.68	0.47
1:D:376:LEU:O	1:D:377:ARG:C	2.58	0.47
1:C:577:LEU:CG	1:C:582:MET:HE3	2.45	0.47
1:D:466:ALA:CB	1:D:482:MET:HE1	2.45	0.47
1:B:528:LEU:CD1	1:B:536:LEU:HD22	2.45	0.46
1:D:322:CYS:HB2	1:D:387:HIS:CG	2.51	0.46
1:C:381:ARG:HG2	1:C:438:ILE:HD12	1.98	0.46
1:B:372:LYS:HE3	1:B:375:ASP:OD2	2.14	0.46
1:B:571:LEU:O	1:B:574:THR:HG22	2.16	0.46
1:B:422:ARG:HH22	1:B:460:PRO:HB3	1.80	0.46
1:B:629:MET:O	1:B:630:ILE:CB	2.63	0.46
1:A:461:GLN:HA	1:A:464:ASN:ND2	2.30	0.46
1:C:571:LEU:C	1:C:574:THR:HG22	2.41	0.46
1:B:459:CYS:HB3	1:B:460:PRO:CD	2.46	0.45
1:B:533:VAL:HG22	2:B:738:HOH:O	2.15	0.45
1:A:614:ARG:HD3	1:C:614:ARG:HD3	1.97	0.45
1:B:464:ASN:O	1:B:468:THR:HG23	2.16	0.45
1:C:412:LYS:O	1:C:415:LYS:HB2	2.17	0.45
1:C:571:LEU:CA	1:C:574:THR:HG22	2.46	0.45
1:D:280:LEU:HB3	1:D:377:ARG:NH2	2.32	0.45
1:D:351:ASN:C	1:D:353:THR:H	2.23	0.45
1:B:370:THR:CG2	2:B:753:HOH:O	2.64	0.45
1:C:593:ILE:O	1:C:597:SER:HB2	2.16	0.45
1:B:469:LEU:HD22	1:B:473:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:PRO:HA	1:C:364:ILE:CG2	2.47	0.45
1:C:459:CYS:N	1:C:460:PRO:HD2	2.32	0.45
1:A:519:GLU:OE1	2:A:702:HOH:O	2.21	0.45
1:B:575:LYS:O	1:B:579:GLU:HB2	2.16	0.45
1:D:577:LEU:HD12	1:D:582:MET:CE	2.43	0.45
1:A:587:GLU:OE1	1:A:587:GLU:HA	2.16	0.45
1:C:533:VAL:HG23	1:C:534:ASP:N	2.32	0.44
1:D:402:LEU:O	1:D:402:LEU:HG	2.16	0.44
1:C:396:ASN:HB3	1:C:399:LEU:H	1.81	0.44
1:C:361:PRO:O	1:C:364:ILE:HG23	2.17	0.44
1:A:571:LEU:C	1:A:574:THR:HG22	2.42	0.44
1:C:393:LEU:HD12	1:C:393:LEU:HA	1.63	0.44
1:C:396:ASN:CB	1:C:399:LEU:HB2	2.42	0.44
1:A:455:ILE:HG23	1:A:489:TRP:CH2	2.53	0.44
1:B:407:LYS:HZ2	1:B:407:LYS:HB3	1.82	0.44
1:C:463:ILE:HG22	1:C:464:ASN:H	1.82	0.44
1:A:498:GLU:OE2	1:A:552:HIS:HE1	2.01	0.44
1:D:290:ASP:HB3	1:D:293:THR:HG22	2.00	0.44
1:B:569:LYS:HB2	1:B:569:LYS:HE2	1.63	0.44
1:D:582:MET:N	1:D:582:MET:HE2	2.33	0.44
1:D:292:MET:HA	1:D:355:ARG:O	2.18	0.43
1:A:293:THR:HG22	2:A:752:HOH:O	2.19	0.43
1:D:395:THR:HG22	2:D:707:HOH:O	2.17	0.43
1:A:506:VAL:O	1:A:510:LEU:HD22	2.18	0.43
1:A:327:ARG:NH1	1:A:386:ASP:OD1	2.51	0.43
1:B:373:THR:HG22	2:B:713:HOH:O	2.19	0.43
1:C:303:LEU:HD12	1:C:303:LEU:HA	1.88	0.43
1:C:510:LEU:HG	1:C:624:ARG:HB2	1.99	0.43
1:D:520:ASP:OD2	1:D:546:ARG:NH1	2.46	0.43
1:C:494:ARG:O	1:C:498:GLU:CG	2.59	0.43
1:D:577:LEU:CG	1:D:582:MET:HE3	2.45	0.43
1:C:452:ALA:O	1:C:455:ILE:HB	2.19	0.43
1:B:373:THR:CG2	1:B:377:ARG:HH12	2.27	0.43
1:C:463:ILE:O	1:C:464:ASN:C	2.61	0.43
1:A:293:THR:CG2	2:A:752:HOH:O	2.66	0.42
1:D:463:ILE:CG2	1:D:464:ASN:N	2.82	0.42
1:D:287:ILE:HD13	1:D:369:MET:HG2	2.01	0.42
1:B:625:LYS:HZ1	1:D:607:ASN:HD21	1.66	0.42
1:C:520:ASP:OD2	1:C:546:ARG:NH1	2.51	0.42
1:B:466:ALA:HB2	1:B:482:MET:HE1	1.99	0.42
1:C:327:ARG:CD	1:C:382:LYS:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ASN:HB3	1:C:399:LEU:CB	2.47	0.42
1:D:393:LEU:O	1:D:394:GLU:C	2.62	0.42
1:C:520:ASP:HB3	1:C:543:ILE:CG1	2.49	0.42
1:D:394:GLU:OE2	1:D:394:GLU:HA	2.19	0.42
1:D:370:THR:CG2	1:D:374:ARG:HH22	2.25	0.42
1:D:281:ASN:HD21	1:D:440:ASN:ND2	2.18	0.42
1:D:422:ARG:HH22	1:D:460:PRO:HB3	1.85	0.42
1:B:388:ILE:HG23	1:B:392:PHE:CD2	2.54	0.42
1:C:360:ASP:O	1:C:364:ILE:HG22	2.20	0.42
1:D:606:GLU:HG3	1:D:607:ASN:N	2.34	0.42
1:D:276:LEU:HB3	1:D:437:SER:O	2.20	0.41
1:C:371:LYS:O	1:C:374:ARG:HB3	2.20	0.41
1:A:446:LYS:O	1:A:450:MET:HG3	2.20	0.41
1:A:582:MET:HB2	1:A:582:MET:HE2	1.86	0.41
1:A:331:ILE:HD11	1:A:383:ALA:HB2	2.02	0.41
1:A:370:THR:HG23	1:A:374:ARG:NH1	2.36	0.41
1:D:571:LEU:HD12	1:D:571:LEU:HA	1.90	0.41
1:A:349:TYR:C	1:A:351:ASN:O	2.64	0.41
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.90	0.41
1:A:406:ALA:HA	1:A:470:ALA:HB2	2.02	0.41
1:A:606:GLU:CD	1:C:624:ARG:HH22	2.29	0.41
1:C:426:ASN:O	1:C:430:GLU:HG3	2.19	0.41
1:D:631:ARG:NH1	1:D:631:ARG:CG	2.83	0.41
1:A:327:ARG:HH11	1:A:386:ASP:CG	2.29	0.41
1:B:303:LEU:HD12	1:B:303:LEU:HA	1.87	0.41
1:A:463:ILE:CG2	1:A:464:ASN:N	2.84	0.41
1:A:621:ARG:NH2	1:C:607:ASN:OD1	2.53	0.41
1:B:327:ARG:NH2	1:B:515:ASN:ND2	2.45	0.41
1:C:418:ALA:HB1	1:C:463:ILE:CG1	2.51	0.41
1:C:445:VAL:O	1:C:449:ARG:HG3	2.21	0.41
1:D:307:LEU:O	1:D:310:ILE:HB	2.21	0.41
1:D:496:LEU:HD12	1:D:496:LEU:O	2.21	0.41
1:C:533:VAL:CG2	1:C:534:ASP:N	2.83	0.41
1:D:351:ASN:C	1:D:353:THR:N	2.79	0.41
1:D:415:LYS:HA	1:D:415:LYS:HD3	1.82	0.41
1:A:456:ASP:O	1:A:460:PRO:HD2	2.21	0.40
1:D:631:ARG:HH11	1:D:631:ARG:CG	2.29	0.40
1:A:290:ASP:HA	1:A:291:PRO:HD3	1.91	0.40
1:B:410:ASN:O	1:B:414:VAL:HG23	2.21	0.40
1:B:445:VAL:O	1:B:449:ARG:HG3	2.21	0.40
1:A:317:MET:HB2	1:A:317:MET:HE2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:GLU:OE2	1:B:568:GLU:CA	2.69	0.40
1:D:355:ARG:HG2	1:D:355:ARG:NH1	2.37	0.40
1:A:569:LYS:HE3	1:A:569:LYS:HB2	1.95	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	350/375 (93%)	343 (98%)	6 (2%)	1 (0%)	36	45
1	B	352/375 (94%)	347 (99%)	5 (1%)	0	100	100
1	C	357/375 (95%)	347 (97%)	7 (2%)	3 (1%)	16	20
1	D	352/375 (94%)	333 (95%)	15 (4%)	4 (1%)	11	12
All	All	1411/1500 (94%)	1370 (97%)	33 (2%)	8 (1%)	21	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	LYS
1	C	396	ASN
1	C	599	ASN
1	D	360	ASP
1	A	410	ASN
1	C	605	GLU
1	D	410	ASN
1	D	273	ILE

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	295/319 (92%)	253 (86%)	42 (14%)	3	2
1	B	295/319 (92%)	254 (86%)	41 (14%)	3	2
1	C	305/319 (96%)	261 (86%)	44 (14%)	3	2
1	D	296/319 (93%)	253 (86%)	43 (14%)	3	2
All	All	1191/1276 (93%)	1021 (86%)	170 (14%)	3	2

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	LEU
1	A	292	MET
1	A	293	THR
1	A	298	ARG
1	A	303	LEU
1	A	305	GLU
1	A	317	MET
1	A	352	ASN
1	A	360	ASP
1	A	364	ILE
1	A	370	THR
1	A	372	LYS
1	A	373	THR
1	A	380	LEU
1	A	393	LEU
1	A	396	ASN
1	A	399	LEU
1	A	400	LEU
1	A	414	VAL
1	A	415	LYS
1	A	428	LEU
1	A	447	LEU
1	A	448	VAL
1	A	463	ILE

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Mol	Chain	Res	Type
1	A	469	LEU
1	A	476	LYS
1	A	491	LYS
1	A	510	LEU
1	A	523	LYS
1	A	528	LEU
1	A	530	GLU
1	A	550	VAL
1	A	571	LEU
1	A	579	GLU
1	A	584	ARG
1	A	588	GLN
1	A	590	GLU
1	A	604	PHE
1	A	605	GLU
1	A	606	GLU
1	A	624	ARG
1	A	629	MET
1	B	280	LEU
1	B	287	ILE
1	B	293	THR
1	B	302	SER
1	B	303	LEU
1	B	305	GLU
1	B	327	ARG
1	B	330	ARG
1	B	352	ASN
1	B	355	ARG
1	B	360	ASP
1	B	370	THR
1	B	372	LYS
1	B	373	THR
1	B	380	LEU
1	B	393	LEU
1	B	399	LEU
1	B	407	LYS
1	B	415	LYS
1	B	428	LEU
1	B	447	LEU
1	B	448	VAL
1	B	468	THR
1	B	469	LEU

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Mol	Chain	Res	Type
1	B	472	ARG
1	B	505	SER
1	B	510	LEU
1	B	528	LEU
1	B	530	GLU
1	B	550	VAL
1	B	553	ILE
1	B	568	GLU
1	B	569	LYS
1	B	571	LEU
1	B	579	GLU
1	B	584	ARG
1	B	590	GLU
1	B	608	GLU
1	B	615	LEU
1	B	624	ARG
1	B	628	LEU
1	C	280	LEU
1	C	282	GLU
1	C	286	LYS
1	C	303	LEU
1	C	309	SER
1	C	328	ARG
1	C	330	ARG
1	C	355	ARG
1	C	363	ASN
1	C	364	ILE
1	C	370	THR
1	C	372	LYS
1	C	373	THR
1	C	380	LEU
1	C	382	LYS
1	C	393	LEU
1	C	395	THR
1	C	397	VAL
1	C	399	LEU
1	C	411	GLU
1	C	415	LYS
1	C	419	GLN
1	C	427	LYS
1	C	428	LEU
1	C	447	LEU

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Mol	Chain	Res	Type
1	C	463	ILE
1	C	464	ASN
1	C	469	LEU
1	C	476	LYS
1	C	480	ASP
1	C	488	GLN
1	C	498	GLU
1	C	510	LEU
1	C	523	LYS
1	C	528	LEU
1	C	550	VAL
1	C	553	ILE
1	C	568	GLU
1	C	571	LEU
1	C	575	LYS
1	C	597	SER
1	C	599	ASN
1	C	605	GLU
1	C	608	GLU
1	D	271	THR
1	D	280	LEU
1	D	287	ILE
1	D	292	MET
1	D	298	ARG
1	D	303	LEU
1	D	312	SER
1	D	316	LEU
1	D	350	MET
1	D	352	ASN
1	D	353	THR
1	D	358	LYS
1	D	360	ASP
1	D	364	ILE
1	D	368	LYS
1	D	370	THR
1	D	372	LYS
1	D	373	THR
1	D	380	LEU
1	D	393	LEU
1	D	399	LEU
1	D	401	VAL
1	D	408	SER

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Mol	Chain	Res	Type
1	D	413	GLU
1	D	415	LYS
1	D	447	LEU
1	D	448	VAL
1	D	454	GLN
1	D	463	ILE
1	D	469	LEU
1	D	475	SER
1	D	486	LYS
1	D	510	LEU
1	D	528	LEU
1	D	550	VAL
1	D	569	LYS
1	D	571	LEU
1	D	572	GLU
1	D	574	THR
1	D	584	ARG
1	D	588	GLN
1	D	624	ARG
1	D	628	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	A	419	GLN
1	A	464	ASN
1	A	479	GLN
1	A	481	ASN
1	A	522	ASN
1	A	552	HIS
1	A	555	ASN
1	A	560	ASN
1	A	607	ASN
1	B	351	ASN
1	B	363	ASN
1	B	419	GLN
1	B	461	GLN
1	B	515	ASN
1	B	522	ASN
1	B	555	ASN
1	B	560	ASN

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Mol	Chain	Res	Type
1	C	363	ASN
1	C	396	ASN
1	C	419	GLN
1	C	440	ASN
1	C	479	GLN
1	C	492	GLN
1	C	522	ASN
1	C	552	HIS
1	C	555	ASN
1	C	588	GLN
1	D	363	ASN
1	D	424	HIS
1	D	440	ASN
1	D	454	GLN
1	D	461	GLN
1	D	479	GLN
1	D	515	ASN
1	D	522	ASN
1	D	552	HIS
1	D	555	ASN
1	D	560	ASN
1	D	607	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](#)

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 [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	354/375 (94%)	-0.27	6 (1%) 69 71	18, 36, 70, 89	0
1	B	356/375 (94%)	-0.34	6 (1%) 69 71	19, 35, 62, 88	0
1	C	359/375 (95%)	-0.12	8 (2%) 62 64	24, 43, 78, 102	0
1	D	356/375 (94%)	0.42	32 (8%) 15 13	26, 59, 128, 159	0
All	All	1425/1500 (95%)	-0.08	52 (3%) 46 46	18, 41, 88, 159	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	394	GLU	5.2
1	C	600	VAL	4.4
1	B	271	THR	4.4
1	B	410	ASN	4.4
1	D	297	ALA	4.3
1	D	299	PHE	4.3
1	D	358	LYS	4.0
1	D	271	THR	3.9
1	D	292	MET	3.9
1	C	603	PRO	3.8
1	A	604	PHE	3.5
1	D	360	ASP	3.5
1	D	463	ILE	3.3
1	A	598	ALA	3.1
1	D	407	LYS	3.1
1	B	630	ILE	3.1
1	D	349	TYR	3.0
1	D	298	ARG	3.0
1	D	599	ASN	3.0
1	D	289	LEU	3.0
1	A	410	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	601	PRO	2.9
1	D	361	PRO	2.9
1	C	604	PHE	2.9
1	B	599	ASN	2.9
1	D	272	GLY	2.9
1	D	598	ALA	2.8
1	D	364	ILE	2.8
1	C	271	THR	2.8
1	D	355	ARG	2.7
1	D	288	ILE	2.7
1	D	354	GLY	2.6
1	B	396	ASN	2.6
1	D	476	LYS	2.6
1	B	600	VAL	2.5
1	D	294	PHE	2.5
1	D	363	ASN	2.5
1	A	271	THR	2.5
1	D	471	ALA	2.4
1	D	286	LYS	2.4
1	D	477	VAL	2.3
1	D	362	LEU	2.3
1	D	356	LYS	2.2
1	D	290	ASP	2.2
1	D	293	THR	2.2
1	D	350	MET	2.2
1	A	408	SER	2.1
1	C	602	GLN	2.1
1	D	631	ARG	2.1
1	D	470	ALA	2.0
1	A	417	TYR	2.0
1	C	395	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.