



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:14 PM UTC

PDB ID : 4HYY / pdb_00004hyy
Title : Filament of octameric rings of DMC1 recombinase from Homo sapiens
Authors : Du, L.; Luo, Y.
Deposited on : 2012-11-14
Resolution : 2.60 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

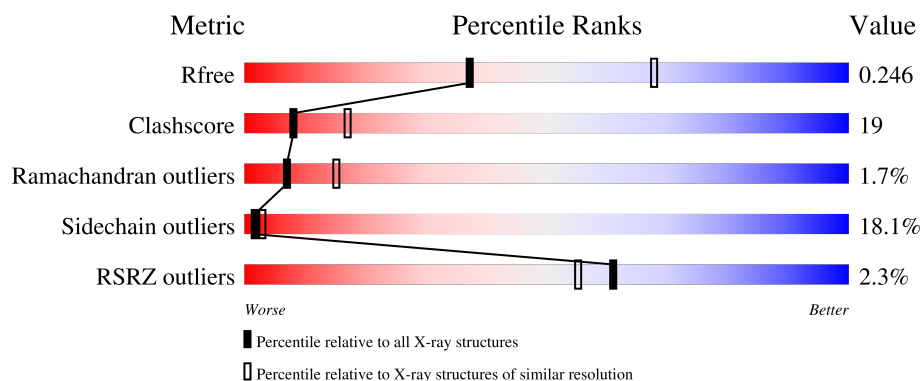
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	265	2% 57% 26% 8% 9%
1	B	265	2% 53% 29% 9% 9%
1	C	265	0% 54% 29% 7% 9%
1	D	265	4% 52% 28% 9% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7632 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 Meiotic recombination protein DMC1/LIM15 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1884	1193	327	356	8			
1	B	241	Total	C	N	O	S	0	0	0
			1884	1193	327	356	8			
1	C	241	Total	C	N	O	S	0	0	0
			1884	1193	327	356	8			
1	D	241	Total	C	N	O	S	0	0	0
			1884	1193	327	356	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	LEU	-	expression tag	UNP Q14565
A	342	GLU	-	expression tag	UNP Q14565
A	343	HIS	-	expression tag	UNP Q14565
A	344	HIS	-	expression tag	UNP Q14565
A	345	HIS	-	expression tag	UNP Q14565
A	346	HIS	-	expression tag	UNP Q14565
A	347	HIS	-	expression tag	UNP Q14565
A	348	HIS	-	expression tag	UNP Q14565
B	341	LEU	-	expression tag	UNP Q14565
B	342	GLU	-	expression tag	UNP Q14565
B	343	HIS	-	expression tag	UNP Q14565
B	344	HIS	-	expression tag	UNP Q14565
B	345	HIS	-	expression tag	UNP Q14565
B	346	HIS	-	expression tag	UNP Q14565
B	347	HIS	-	expression tag	UNP Q14565
B	348	HIS	-	expression tag	UNP Q14565
C	341	LEU	-	expression tag	UNP Q14565
C	342	GLU	-	expression tag	UNP Q14565
C	343	HIS	-	expression tag	UNP Q14565
C	344	HIS	-	expression tag	UNP Q14565
C	345	HIS	-	expression tag	UNP Q14565

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Chain	Residue	Modelled	Actual	Comment	Reference
C	346	HIS	-	expression tag	UNP Q14565
C	347	HIS	-	expression tag	UNP Q14565
C	348	HIS	-	expression tag	UNP Q14565
D	341	LEU	-	expression tag	UNP Q14565
D	342	GLU	-	expression tag	UNP Q14565
D	343	HIS	-	expression tag	UNP Q14565
D	344	HIS	-	expression tag	UNP Q14565
D	345	HIS	-	expression tag	UNP Q14565
D	346	HIS	-	expression tag	UNP Q14565
D	347	HIS	-	expression tag	UNP Q14565
D	348	HIS	-	expression tag	UNP Q14565

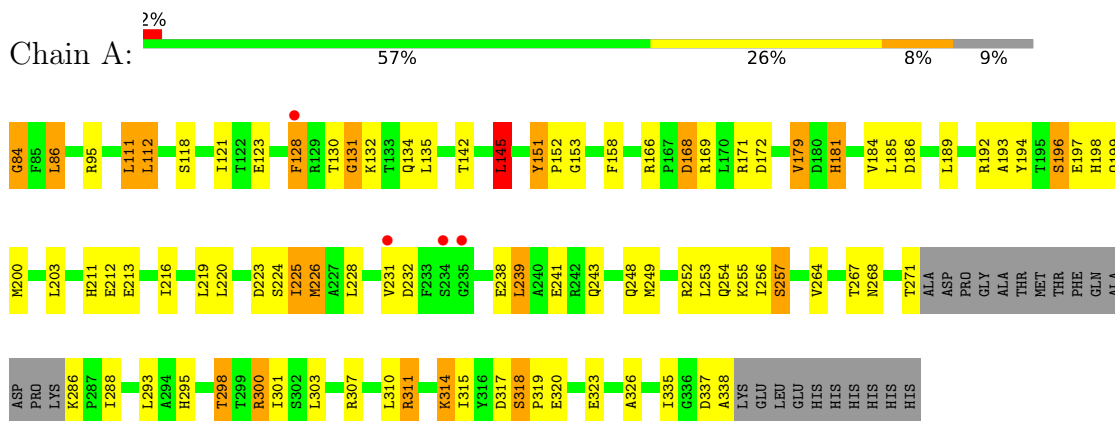
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	22	Total O 22 22	0	0
2	C	29	Total O 29 29	0	0
2	D	16	Total O 16 16	0	0

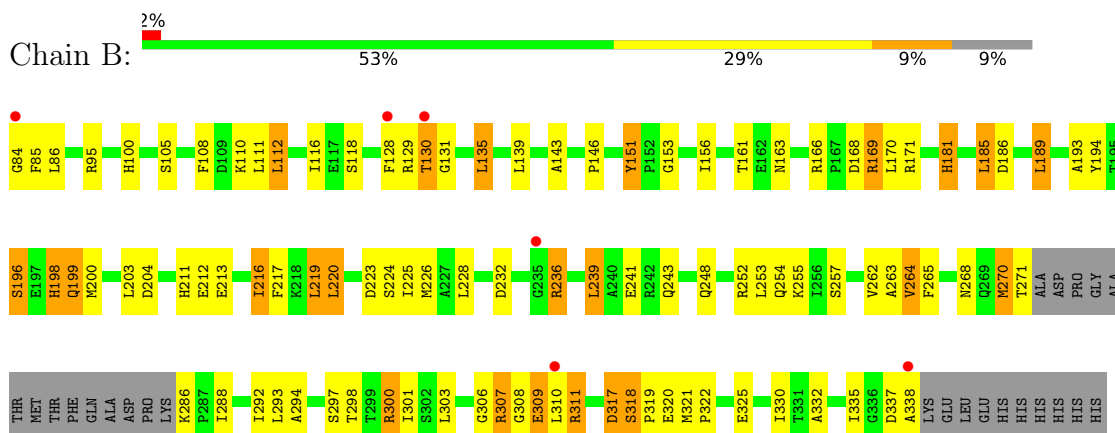
3 Residue-property plots

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.

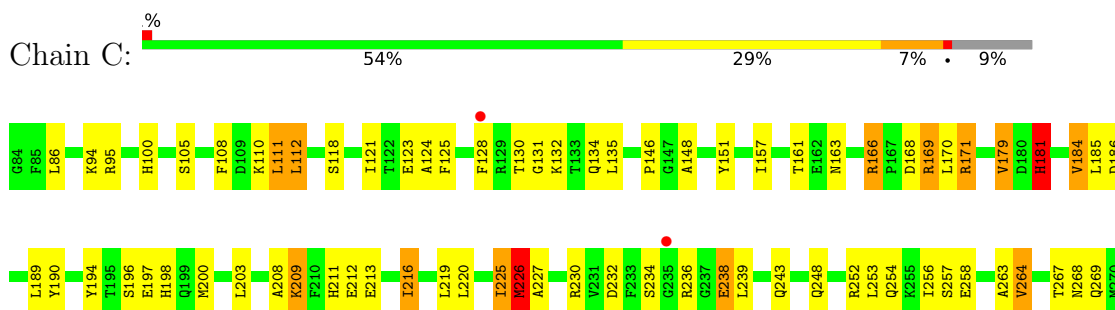
- Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog

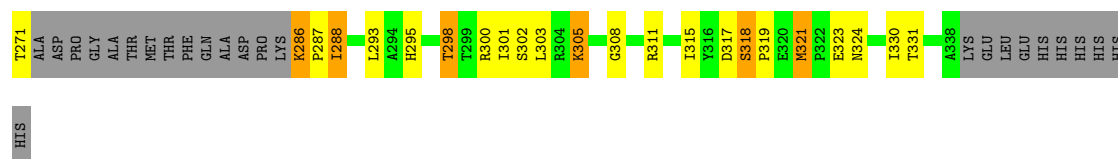


- Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog

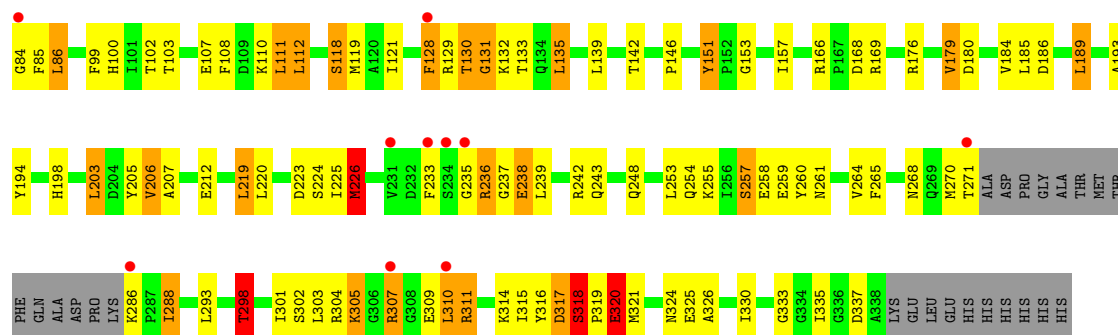


- Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog





- Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	124.00Å 124.00Å 91.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.45 – 2.60 47.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.45-2.60) 96.2 (47.45-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.179 , 0.246 0.178 , 0.246	Depositor DCC
R_{free} test set	2157 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.072 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7632	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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	1.10	3/1917 (0.2%)	1.24	11/2579 (0.4%)
1	B	1.05	2/1917 (0.1%)	1.19	6/2579 (0.2%)
1	C	1.02	2/1917 (0.1%)	1.21	10/2579 (0.4%)
1	D	1.02	1/1917 (0.1%)	1.25	12/2579 (0.5%)
All	All	1.05	8/7668 (0.1%)	1.22	39/10316 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	84	GLY	N-CA	5.73	1.54	1.45
1	B	84	GLY	N-CA	5.70	1.54	1.45
1	A	295	HIS	CE1-NE2	5.70	1.38	1.32
1	B	198	HIS	CG-CD2	5.42	1.41	1.35
1	A	84	GLY	N-CA	5.38	1.54	1.45
1	A	211	HIS	CG-CD2	5.27	1.41	1.35
1	C	181	HIS	CG-CD2	5.15	1.41	1.35
1	C	295	HIS	CE1-NE2	5.00	1.37	1.32

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	LEU	CA-C-N	-9.07	110.42	119.76
1	A	145	LEU	C-N-CA	-9.07	110.42	119.76
1	D	130	THR	N-CA-C	8.91	122.03	110.53
1	C	298	THR	CB-CA-C	7.88	122.31	109.07
1	D	298	THR	CB-CA-C	7.71	123.33	109.29
1	D	236	ARG	N-CA-C	7.57	120.05	109.15
1	C	171	ARG	CB-CA-C	7.19	122.37	109.29
1	C	128	PHE	N-CA-C	7.02	119.59	111.02
1	C	226	MET	CB-CA-C	-6.83	98.06	109.27
1	B	161	THR	N-CA-C	-6.83	104.63	114.12
1	D	225	ILE	N-CA-C	6.75	117.51	110.62
1	C	225	ILE	N-CA-C	6.73	117.52	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ILE	N-CA-C	6.69	117.44	110.62
1	C	209	LYS	N-CA-C	-6.50	104.23	111.71
1	D	129	ARG	N-CA-C	-6.24	104.36	112.23
1	A	168	ASP	N-CA-C	6.17	118.00	111.28
1	A	225	ILE	N-CA-C	6.10	117.57	110.62
1	A	153	GLY	N-CA-C	-6.06	105.14	112.48
1	B	151	TYR	CA-C-N	6.02	125.72	119.64
1	B	151	TYR	C-N-CA	6.02	125.72	119.64
1	A	95	ARG	CG-CD-NE	-5.98	98.84	112.00
1	D	226	MET	CB-CA-C	-5.64	100.02	109.27
1	A	326	ALA	N-CA-C	5.62	117.94	109.23
1	D	153	GLY	N-CA-C	-5.53	106.10	112.29
1	D	235	GLY	N-CA-C	-5.46	100.24	113.18
1	D	205	TYR	N-CA-C	5.43	116.89	111.07
1	C	161	THR	N-CA-C	-5.43	106.24	112.92
1	B	95	ARG	N-CA-C	5.43	117.95	111.71
1	B	199	GLN	N-CA-C	-5.41	105.47	111.36
1	A	226	MET	CB-CG-SD	-5.37	96.59	112.70
1	A	231	VAL	N-CA-C	5.36	115.56	110.42
1	D	206	VAL	N-CA-C	5.35	115.80	110.23
1	A	151	TYR	CA-C-N	5.29	124.99	119.64
1	A	151	TYR	C-N-CA	5.29	124.99	119.64
1	D	151	TYR	CA-C-N	5.21	124.90	119.64
1	D	151	TYR	C-N-CA	5.21	124.90	119.64
1	C	170	LEU	CA-C-N	-5.15	113.02	121.92
1	C	170	LEU	C-N-CA	-5.15	113.02	121.92
1	C	298	THR	N-CA-C	-5.06	107.49	113.97

There are no chirality outliers.

There are no planarity outliers.

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	1884	0	1870	71	0
1	B	1884	0	1870	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1884	0	1870	66	0
1	D	1884	0	1870	82	0
2	A	29	0	0	11	0
2	B	22	0	0	8	0
2	C	29	0	0	10	0
2	D	16	0	0	5	0
All	All	7632	0	7480	292	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 19.

All (292) 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:318:SER:HB3	1:B:319:PRO:HA	1.22	1.15
2:A:428:HOH:O	1:D:212:GLU:HG3	1.49	1.12
1:C:130:THR:HG21	1:C:303:LEU:HB3	1.19	1.12
1:C:318:SER:HB3	1:C:319:PRO:HA	1.21	1.11
1:A:318:SER:HB3	1:A:319:PRO:CA	1.80	1.11
1:C:212:GLU:HG2	2:C:429:HOH:O	1.49	1.10
1:B:311:ARG:HG2	1:B:311:ARG:HH11	0.99	1.08
1:A:318:SER:HB3	1:A:319:PRO:HA	1.11	1.06
1:D:318:SER:HB3	1:D:319:PRO:HA	1.31	1.04
1:B:318:SER:HB3	1:B:319:PRO:CA	1.89	1.02
1:D:130:THR:HG21	1:D:303:LEU:HB3	1.41	1.01
1:B:286:LYS:N	2:B:406:HOH:O	1.92	1.00
1:B:169:ARG:HG3	1:B:169:ARG:HH11	1.28	0.97
1:D:318:SER:HB3	1:D:319:PRO:CA	1.94	0.97
1:A:311:ARG:CG	1:A:311:ARG:HH11	1.77	0.97
1:B:130:THR:HG21	1:B:303:LEU:HB3	1.45	0.97
1:C:286:LYS:N	2:C:403:HOH:O	1.97	0.96
1:C:169:ARG:HG3	1:C:169:ARG:HH11	1.33	0.94
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.31	0.94
1:A:311:ARG:HH11	1:A:311:ARG:HG2	1.29	0.92
1:B:311:ARG:HG2	1:B:311:ARG:NH1	1.77	0.92
1:D:100:HIS:HD2	2:D:408:HOH:O	1.52	0.92
1:B:100:HIS:HD2	2:B:416:HOH:O	1.52	0.92
1:C:130:THR:HG21	1:C:303:LEU:CB	1.99	0.92
1:A:318:SER:CB	1:A:319:PRO:HA	1.99	0.91
1:B:130:THR:HG22	1:B:131:GLY:H	1.36	0.91
1:A:197:GLU:HG3	2:A:404:HOH:O	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:HG21	1:A:303:LEU:HB3	1.54	0.89
1:C:130:THR:CG2	1:C:303:LEU:HB3	2.04	0.87
1:C:318:SER:HB3	1:C:319:PRO:CA	2.05	0.87
1:C:216:ILE:HD11	2:C:424:HOH:O	1.74	0.87
1:D:130:THR:HG22	1:D:131:GLY:N	1.88	0.85
1:A:130:THR:HA	1:A:311:ARG:HH12	1.41	0.85
1:D:239:LEU:O	1:D:243:GLN:HG2	1.76	0.85
1:A:254:GLN:O	1:A:257:SER:HB3	1.78	0.84
1:D:128:PHE:HZ	1:D:133:THR:HG1	0.85	0.84
1:B:216:ILE:HD12	1:B:216:ILE:H	1.41	0.83
1:D:128:PHE:HZ	1:D:133:THR:OG1	1.61	0.83
1:C:318:SER:CB	1:C:319:PRO:HA	2.06	0.83
1:A:142:THR:HA	1:A:145:LEU:HD22	1.62	0.81
1:A:130:THR:HG21	1:A:303:LEU:CB	2.11	0.81
1:C:194:TYR:H	1:C:198:HIS:HD2	1.28	0.80
1:A:239:LEU:O	1:A:243:GLN:HG2	1.83	0.79
1:C:112:LEU:HD11	1:C:301:ILE:HD11	1.66	0.78
1:C:171:ARG:HE	1:C:181:HIS:HB2	1.48	0.77
1:A:194:TYR:H	1:A:198:HIS:HD2	1.30	0.77
1:D:130:THR:HA	1:D:311:ARG:HE	1.49	0.77
1:B:311:ARG:HH11	1:B:311:ARG:CG	1.88	0.77
1:D:130:THR:HG22	1:D:131:GLY:H	1.46	0.77
1:D:121:ILE:H	1:D:298:THR:HG23	1.49	0.77
1:B:171:ARG:HG2	1:B:181:HIS:HB3	1.67	0.76
1:B:239:LEU:O	1:B:243:GLN:HG2	1.85	0.76
1:B:298:THR:HG23	2:B:405:HOH:O	1.85	0.75
1:A:216:ILE:HD11	2:A:403:HOH:O	1.85	0.75
1:D:233:PHE:HB2	1:D:242:ARG:HB2	1.69	0.75
1:D:314:LYS:HD3	1:D:325:GLU:HG2	1.69	0.75
1:C:239:LEU:O	1:C:243:GLN:HG2	1.87	0.75
1:C:319:PRO:HD2	1:C:324:ASN:ND2	2.02	0.74
1:A:200:MET:HE1	1:A:252:ARG:HG3	1.69	0.73
1:D:311:ARG:HH11	1:D:311:ARG:CG	2.01	0.73
1:B:130:THR:HG21	1:B:303:LEU:CB	2.18	0.73
1:B:131:GLY:N	1:B:311:ARG:HH12	1.87	0.72
1:D:307:ARG:O	1:D:310:LEU:HD13	1.90	0.72
1:B:194:TYR:H	1:B:198:HIS:HD2	1.38	0.71
1:A:130:THR:CG2	1:A:303:LEU:HB3	2.21	0.71
1:B:216:ILE:HD13	1:B:217:PHE:H	1.54	0.71
1:B:169:ARG:HH11	1:B:169:ARG:CG	2.01	0.71
1:C:238:GLU:OE1	1:C:238:GLU:HA	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLU:HB3	1:C:216:ILE:HD12	1.72	0.70
1:A:112:LEU:HD11	1:A:301:ILE:HD11	1.73	0.70
1:B:110:LYS:HG3	1:B:111:LEU:N	2.06	0.69
1:B:254:GLN:O	1:B:257:SER:HB3	1.93	0.69
1:C:226:MET:HE2	1:C:288:ILE:HD13	1.74	0.68
1:A:298:THR:HG21	1:B:163:ASN:HD22	1.59	0.68
1:C:163:ASN:HD22	1:D:298:THR:HG21	1.58	0.68
1:C:254:GLN:O	1:C:257:SER:HB3	1.93	0.68
1:D:194:TYR:H	1:D:198:HIS:HD2	1.39	0.68
1:A:130:THR:HG22	1:A:131:GLY:N	2.09	0.67
1:B:309:GLU:HB2	1:B:330:ILE:HD11	1.77	0.67
1:D:130:THR:CG2	1:D:131:GLY:H	2.09	0.66
1:A:311:ARG:HG2	1:A:311:ARG:NH1	2.07	0.66
1:B:130:THR:CG2	1:B:303:LEU:HB3	2.24	0.66
1:C:111:LEU:HD22	1:C:315:ILE:CD1	2.26	0.65
1:B:338:ALA:HB1	2:B:420:HOH:O	1.96	0.65
1:D:100:HIS:CD2	2:D:408:HOH:O	2.36	0.65
1:B:200:MET:HE1	1:B:252:ARG:HG3	1.79	0.65
1:D:111:LEU:HD22	1:D:315:ILE:CD1	2.27	0.65
1:C:319:PRO:HD2	1:C:324:ASN:HD21	1.61	0.64
1:B:196:SER:HB2	1:B:232:ASP:OD2	1.97	0.64
1:B:306:GLY:O	1:B:308:GLY:N	2.31	0.64
1:A:310:LEU:C	1:A:311:ARG:HD2	2.22	0.64
1:A:130:THR:HG22	1:A:131:GLY:H	1.62	0.63
1:A:84:GLY:O	2:A:419:HOH:O	2.16	0.62
1:C:100:HIS:HD2	2:C:406:HOH:O	1.80	0.62
1:C:252:ARG:O	1:C:256:ILE:HG13	1.98	0.62
1:D:307:ARG:HH11	1:D:307:ARG:HB2	1.64	0.62
1:B:131:GLY:H	1:B:311:ARG:HH12	1.45	0.62
1:A:213:GLU:N	2:A:403:HOH:O	2.31	0.62
1:A:123:GLU:OE1	1:A:300:ARG:HD2	2.00	0.62
1:D:318:SER:HB3	1:D:319:PRO:C	2.24	0.61
1:A:130:THR:HA	1:A:311:ARG:NH1	2.12	0.61
1:B:216:ILE:HD13	1:B:217:PHE:N	2.16	0.61
1:D:111:LEU:HD22	1:D:315:ILE:HD11	1.83	0.61
1:B:130:THR:HG22	1:B:131:GLY:N	2.13	0.60
1:C:125:PHE:HB3	1:C:268:ASN:HB3	1.82	0.60
1:D:112:LEU:HD11	1:D:301:ILE:HD11	1.84	0.60
1:A:172:ASP:HB3	2:A:413:HOH:O	2.01	0.59
1:C:230:ARG:O	1:C:234:SER:HB3	2.02	0.59
1:D:233:PHE:CB	1:D:242:ARG:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:TYR:H	1:C:198:HIS:CD2	2.17	0.59
1:C:123:GLU:OE1	1:C:300:ARG:HD2	2.02	0.59
1:A:225:ILE:HG22	1:A:267:THR:O	2.03	0.59
1:C:186:ASP:HB3	2:C:419:HOH:O	2.02	0.58
1:A:298:THR:CG2	2:A:402:HOH:O	2.51	0.58
1:A:171:ARG:HG2	1:A:181:HIS:HB3	1.84	0.58
1:B:216:ILE:HD12	1:B:216:ILE:N	2.16	0.57
1:D:268:ASN:ND2	2:D:405:HOH:O	2.34	0.57
1:D:311:ARG:CG	1:D:311:ARG:NH1	2.65	0.57
1:C:323:GLU:HA	2:C:423:HOH:O	2.03	0.57
1:D:319:PRO:O	1:D:320:GLU:HB2	2.04	0.57
1:C:110:LYS:HD3	2:C:418:HOH:O	2.05	0.57
1:D:238:GLU:O	1:D:238:GLU:HG2	2.05	0.56
1:D:318:SER:CB	1:D:319:PRO:HA	2.20	0.56
1:B:105:SER:HB3	1:B:108:PHE:HB2	1.86	0.56
1:D:111:LEU:CD2	1:D:315:ILE:CD1	2.84	0.56
1:B:204:ASP:OD1	1:B:252:ARG:NH2	2.35	0.55
1:B:216:ILE:CD1	1:B:217:PHE:H	2.19	0.55
1:C:130:THR:HG22	1:C:131:GLY:N	2.22	0.55
1:A:194:TYR:H	1:A:198:HIS:CD2	2.20	0.54
1:C:111:LEU:HD22	1:C:315:ILE:HD13	1.89	0.54
1:A:199:GLN:HE21	1:A:228:LEU:HD12	1.71	0.54
1:C:148:ALA:HA	2:C:407:HOH:O	2.08	0.53
1:B:171:ARG:HG2	1:B:181:HIS:CB	2.36	0.53
1:B:292:ILE:HD12	2:B:421:HOH:O	2.08	0.53
1:C:163:ASN:O	1:C:166:ARG:NH2	2.42	0.53
1:C:169:ARG:HH11	1:C:169:ARG:CG	2.13	0.53
1:D:316:TYR:O	1:D:317:ASP:HB2	2.08	0.53
1:A:318:SER:HB3	1:A:319:PRO:C	2.33	0.53
1:C:286:LYS:HG2	1:C:287:PRO:HD2	1.92	0.52
1:C:226:MET:O	1:C:227:ALA:C	2.50	0.52
1:C:134:GLN:HE22	1:C:169:ARG:NH1	2.07	0.52
1:D:146:PRO:HA	1:D:151:TYR:O	2.09	0.52
1:A:225:ILE:HD11	1:A:249:MET:HE3	1.91	0.52
1:D:305:LYS:HA	1:D:311:ARG:HG2	1.92	0.52
1:A:123:GLU:OE1	1:A:300:ARG:CD	2.58	0.51
1:C:130:THR:HG22	1:C:131:GLY:H	1.75	0.51
1:B:199:GLN:HE21	1:B:228:LEU:HD12	1.74	0.51
1:B:307:ARG:HB3	1:B:310:LEU:HD13	1.92	0.51
1:D:119:MET:HG2	1:D:258:GLU:HA	1.92	0.51
1:C:121:ILE:HG23	1:C:264:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLN:NE2	2:B:411:HOH:O	2.43	0.51
1:C:146:PRO:HA	1:C:151:TYR:O	2.11	0.51
1:D:128:PHE:HZ	1:D:133:THR:CB	2.23	0.51
1:B:216:ILE:H	1:B:216:ILE:CD1	2.17	0.51
1:D:194:TYR:H	1:D:198:HIS:CD2	2.25	0.51
1:A:311:ARG:CG	1:A:311:ARG:NH1	2.48	0.50
1:D:135:LEU:HD13	1:D:265:PHE:CZ	2.46	0.50
1:A:181:HIS:ND1	1:A:181:HIS:N	2.58	0.50
1:D:102:THR:HG23	1:D:142:THR:HB	1.93	0.50
1:B:337:ASP:O	1:B:338:ALA:C	2.55	0.50
1:D:236:ARG:HB2	1:D:239:LEU:HG	1.94	0.50
1:B:270:MET:HE3	2:B:422:HOH:O	2.11	0.49
1:D:318:SER:CB	1:D:319:PRO:CA	2.78	0.49
1:B:146:PRO:HA	1:B:151:TYR:O	2.12	0.49
1:B:271:THR:HG23	1:B:288:ILE:HG22	1.94	0.49
1:D:130:THR:HG23	1:D:311:ARG:HD3	1.94	0.48
1:A:86:LEU:HD23	1:A:86:LEU:H	1.77	0.48
1:A:311:ARG:HH11	1:A:311:ARG:HG3	1.69	0.48
1:C:171:ARG:NE	1:C:181:HIS:HB2	2.23	0.48
1:A:130:THR:HG21	1:A:303:LEU:HB2	1.95	0.48
1:C:169:ARG:HG3	1:C:169:ARG:NH1	2.11	0.48
1:A:298:THR:HG21	1:B:163:ASN:ND2	2.25	0.48
1:C:134:GLN:HE22	1:C:169:ARG:HH12	1.59	0.48
1:D:307:ARG:HB2	1:D:307:ARG:NH1	2.28	0.47
1:A:223:ASP:HA	1:A:224:SER:HA	1.74	0.47
1:B:211:HIS:CD2	2:B:407:HOH:O	2.68	0.47
1:A:196:SER:HB2	1:A:232:ASP:OD2	2.15	0.47
1:B:151:TYR:CE2	1:B:153:GLY:HA2	2.50	0.47
1:D:226:MET:HE2	1:D:288:ILE:HD13	1.97	0.47
1:C:318:SER:CB	1:C:319:PRO:CA	2.78	0.47
1:B:311:ARG:NH1	1:B:311:ARG:CG	2.57	0.47
1:B:112:LEU:HD11	1:B:301:ILE:HD11	1.97	0.46
1:D:130:THR:CG2	1:D:131:GLY:N	2.59	0.46
1:A:314:LYS:NZ	1:A:320:GLU:OE2	2.48	0.46
1:B:139:LEU:HB3	1:B:219:LEU:HD11	1.98	0.46
1:D:226:MET:HB2	2:D:405:HOH:O	2.14	0.46
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.79	0.46
1:A:128:PHE:CD1	1:A:128:PHE:N	2.82	0.46
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.68	0.46
1:D:176:ARG:HD2	1:D:333:GLY:O	2.15	0.46
1:B:143:ALA:HB3	1:B:156:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:NH2	1:B:332:ALA:O	2.47	0.46
1:A:84:GLY:CA	2:A:419:HOH:O	2.63	0.46
1:A:134:GLN:OE1	1:A:169:ARG:NH1	2.49	0.46
1:B:213:GLU:O	1:B:216:ILE:HD11	2.16	0.46
1:C:118:SER:HA	1:C:263:ALA:HA	1.97	0.46
1:A:158:PHE:C	1:A:158:PHE:CD2	2.94	0.46
1:D:193:ALA:HA	1:D:198:HIS:CD2	2.51	0.46
1:C:208:ALA:O	1:C:209:LYS:C	2.57	0.46
1:B:319:PRO:C	1:B:321:MET:H	2.24	0.45
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.83	0.45
1:C:169:ARG:HD2	1:C:169:ARG:HA	1.82	0.45
1:D:206:VAL:O	1:D:207:ALA:C	2.57	0.45
1:A:337:ASP:O	1:A:338:ALA:C	2.58	0.45
1:B:116:ILE:HG22	1:B:263:ALA:HB1	1.99	0.45
1:D:86:LEU:HD23	1:D:86:LEU:H	1.81	0.45
1:D:268:ASN:HD21	1:D:288:ILE:HD12	1.80	0.45
1:A:131:GLY:O	1:A:132:LYS:C	2.59	0.45
1:D:107:GLU:HB3	1:D:326:ALA:HB1	1.98	0.45
1:B:86:LEU:N	1:B:86:LEU:HD23	2.32	0.45
1:B:223:ASP:HA	1:B:224:SER:HA	1.67	0.45
1:D:320:GLU:HB3	1:D:321:MET:HE2	1.99	0.45
1:D:103:THR:OG1	1:D:108:PHE:HB3	2.17	0.45
1:B:85:PHE:CD1	1:B:85:PHE:N	2.85	0.45
1:B:189:LEU:HD23	1:B:217:PHE:CZ	2.51	0.45
1:B:294:ALA:HB2	1:B:300:ARG:HH21	1.82	0.45
1:A:200:MET:HE1	1:A:252:ARG:CG	2.44	0.44
1:C:94:LYS:NZ	1:C:258:GLU:O	2.50	0.44
1:C:196:SER:HB2	1:C:232:ASP:OD2	2.17	0.44
1:C:321:MET:HB3	1:C:323:GLU:HG2	1.99	0.44
1:A:111:LEU:HD13	1:A:315:ILE:HD12	1.99	0.44
1:D:131:GLY:O	1:D:135:LEU:HB2	2.18	0.44
2:A:428:HOH:O	1:D:212:GLU:CG	2.30	0.44
1:D:318:SER:OG	1:D:320:GLU:N	2.51	0.44
1:A:193:ALA:HA	1:A:198:HIS:CD2	2.53	0.44
1:C:197:GLU:HB2	2:C:410:HOH:O	2.17	0.44
1:D:319:PRO:HD2	1:D:324:ASN:ND2	2.33	0.44
1:D:189:LEU:HD12	1:D:189:LEU:HA	1.87	0.44
1:A:268:ASN:HD21	1:A:288:ILE:HG13	1.82	0.44
1:A:286:LYS:N	2:A:423:HOH:O	2.51	0.44
1:A:268:ASN:HD21	1:A:288:ILE:CG1	2.30	0.43
1:A:310:LEU:O	1:A:311:ARG:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:SER:HB3	1:C:108:PHE:HB2	2.00	0.43
1:A:179:VAL:CG1	1:A:184:VAL:HG23	2.47	0.43
1:D:121:ILE:N	1:D:298:THR:HG23	2.27	0.43
1:B:253:LEU:HA	1:B:253:LEU:HD23	1.72	0.43
1:D:132:LYS:HE3	1:D:132:LYS:HB2	1.83	0.43
1:B:118:SER:HA	1:B:263:ALA:HA	2.00	0.43
1:D:179:VAL:HG12	1:D:180:ASP:H	1.84	0.43
1:B:226:MET:HE2	1:B:226:MET:HB3	1.84	0.43
1:D:253:LEU:HD23	1:D:253:LEU:HA	1.80	0.43
1:B:317:ASP:O	1:B:318:SER:O	2.37	0.43
1:C:190:TYR:O	1:D:85:PHE:HA	2.19	0.43
1:C:225:ILE:HG23	1:C:226:MET:HG3	2.00	0.42
1:C:226:MET:CE	1:C:288:ILE:HD13	2.47	0.42
1:A:130:THR:CG2	1:A:131:GLY:N	2.79	0.42
1:A:212:GLU:HG3	2:D:411:HOH:O	2.18	0.42
1:A:314:LYS:HE2	1:A:318:SER:HA	2.01	0.42
1:B:220:LEU:HB3	1:B:264:VAL:HB	2.00	0.42
1:C:330:ILE:HD12	1:C:330:ILE:O	2.19	0.42
1:D:118:SER:OG	1:D:261:ASN:OD1	2.37	0.42
1:C:253:LEU:HD23	1:C:253:LEU:HA	1.65	0.42
1:D:238:GLU:O	1:D:238:GLU:CG	2.67	0.42
1:A:151:TYR:HA	1:A:152:PRO:HD3	1.93	0.42
1:A:192:ARG:HH11	1:A:192:ARG:HD2	1.72	0.42
1:A:179:VAL:CG1	1:A:184:VAL:CG2	2.98	0.42
1:B:170:LEU:HD12	1:B:185:LEU:HD12	2.01	0.42
1:C:305:LYS:HB3	1:C:305:LYS:HE2	1.50	0.42
1:B:268:ASN:HD21	1:B:288:ILE:CG1	2.33	0.42
1:B:236:ARG:HA	1:B:239:LEU:HD23	2.02	0.42
1:D:111:LEU:CD2	1:D:315:ILE:HD13	2.49	0.42
1:D:223:ASP:HA	1:D:224:SER:HA	1.77	0.42
1:D:303:LEU:HD23	1:D:303:LEU:HA	1.81	0.42
1:B:330:ILE:H	1:B:330:ILE:HG13	1.76	0.41
1:B:307:ARG:HH11	1:B:307:ARG:HA	1.84	0.41
1:D:130:THR:O	1:D:132:LYS:N	2.54	0.41
1:D:139:LEU:HB3	1:D:219:LEU:HD11	2.03	0.41
1:D:255:LYS:O	1:D:259:GLU:HB2	2.20	0.41
1:A:319:PRO:HB3	2:A:415:HOH:O	2.19	0.41
1:C:179:VAL:CG1	1:C:184:VAL:HG23	2.50	0.41
1:A:194:TYR:N	1:A:198:HIS:HD2	2.10	0.41
1:C:268:ASN:ND2	1:C:269:GLN:H	2.18	0.41
1:B:105:SER:HB3	1:B:108:PHE:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:PHE:CE1	1:D:118:SER:HB2	2.55	0.41
1:A:121:ILE:HD11	1:A:253:LEU:HB3	2.02	0.41
1:A:130:THR:CG2	1:A:131:GLY:H	2.31	0.41
1:B:135:LEU:HD13	1:B:265:PHE:CZ	2.56	0.41
1:B:322:PRO:O	1:B:325:GLU:N	2.46	0.41
1:D:236:ARG:HD2	1:D:239:LEU:HD11	2.03	0.41
1:B:193:ALA:HA	1:B:198:HIS:CD2	2.56	0.40
1:C:132:LYS:HD2	1:C:267:THR:HB	2.03	0.40
1:D:319:PRO:O	1:D:320:GLU:CB	2.69	0.40
1:C:124:ALA:O	1:C:267:THR:HA	2.21	0.40
1:C:130:THR:HG23	1:C:311:ARG:HD2	2.04	0.40
1:C:226:MET:HB2	2:C:401:HOH:O	2.22	0.40
1:D:169:ARG:HG3	1:D:169:ARG:HH11	1.85	0.40
1:D:260:TYR:O	1:D:261:ASN:C	2.65	0.40
1:A:86:LEU:HD23	1:A:86:LEU:N	2.37	0.40
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.71	0.40
1:B:169:ARG:HA	1:B:169:ARG:HD2	1.75	0.40
1:D:111:LEU:HD21	1:D:315:ILE:HD13	2.04	0.40
1:D:254:GLN:O	1:D:257:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/265 (89%)	221 (93%)	11 (5%)	5 (2%)	5	11
1	B	237/265 (89%)	219 (92%)	14 (6%)	4 (2%)	7	15
1	C	237/265 (89%)	230 (97%)	5 (2%)	2 (1%)	16	34
1	D	237/265 (89%)	220 (93%)	12 (5%)	5 (2%)	5	11
All	All	948/1060 (89%)	890 (94%)	42 (4%)	16 (2%)	7	15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	SER
1	B	128	PHE
1	B	307	ARG
1	B	318	SER
1	D	317	ASP
1	D	318	SER
1	A	257	SER
1	B	320	GLU
1	C	318	SER
1	D	131	GLY
1	D	320	GLU
1	A	131	GLY
1	D	237	GLY
1	A	238	GLU
1	C	308	GLY
1	A	256	ILE

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	196/216 (91%)	162 (83%)	34 (17%)	2	3
1	B	196/216 (91%)	164 (84%)	32 (16%)	2	4
1	C	196/216 (91%)	161 (82%)	35 (18%)	2	3
1	D	196/216 (91%)	155 (79%)	41 (21%)	1	2
All	All	784/864 (91%)	642 (82%)	142 (18%)	2	3

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	111	LEU
1	A	112	LEU
1	A	118	SER

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Mol	Chain	Res	Type
1	A	128	PHE
1	A	135	LEU
1	A	145	LEU
1	A	166	ARG
1	A	168	ASP
1	A	179	VAL
1	A	181	HIS
1	A	185	LEU
1	A	186	ASP
1	A	189	LEU
1	A	196	SER
1	A	203	LEU
1	A	219	LEU
1	A	220	LEU
1	A	226	MET
1	A	239	LEU
1	A	241	GLU
1	A	248	GLN
1	A	255	LYS
1	A	264	VAL
1	A	271	THR
1	A	293	LEU
1	A	298	THR
1	A	300	ARG
1	A	307	ARG
1	A	311	ARG
1	A	314	LYS
1	A	317	ASP
1	A	323	GLU
1	A	335	ILE
1	B	112	LEU
1	B	129	ARG
1	B	130	THR
1	B	135	LEU
1	B	166	ARG
1	B	168	ASP
1	B	169	ARG
1	B	181	HIS
1	B	185	LEU
1	B	186	ASP
1	B	189	LEU
1	B	196	SER

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Mol	Chain	Res	Type
1	B	203	LEU
1	B	212	GLU
1	B	216	ILE
1	B	219	LEU
1	B	220	LEU
1	B	236	ARG
1	B	239	LEU
1	B	241	GLU
1	B	248	GLN
1	B	255	LYS
1	B	262	VAL
1	B	264	VAL
1	B	270	MET
1	B	293	LEU
1	B	297	SER
1	B	300	ARG
1	B	309	GLU
1	B	311	ARG
1	B	317	ASP
1	B	335	ILE
1	C	86	LEU
1	C	95	ARG
1	C	111	LEU
1	C	112	LEU
1	C	135	LEU
1	C	157	ILE
1	C	166	ARG
1	C	168	ASP
1	C	169	ARG
1	C	179	VAL
1	C	181	HIS
1	C	184	VAL
1	C	185	LEU
1	C	189	LEU
1	C	200	MET
1	C	203	LEU
1	C	211	HIS
1	C	216	ILE
1	C	219	LEU
1	C	220	LEU
1	C	226	MET
1	C	236	ARG

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Mol	Chain	Res	Type
1	C	238	GLU
1	C	248	GLN
1	C	264	VAL
1	C	271	THR
1	C	286	LYS
1	C	288	ILE
1	C	293	LEU
1	C	298	THR
1	C	302	SER
1	C	305	LYS
1	C	317	ASP
1	C	321	MET
1	C	331	THR
1	D	86	LEU
1	D	110	LYS
1	D	111	LEU
1	D	112	LEU
1	D	118	SER
1	D	128	PHE
1	D	135	LEU
1	D	157	ILE
1	D	166	ARG
1	D	168	ASP
1	D	179	VAL
1	D	184	VAL
1	D	185	LEU
1	D	186	ASP
1	D	189	LEU
1	D	203	LEU
1	D	219	LEU
1	D	220	LEU
1	D	226	MET
1	D	238	GLU
1	D	248	GLN
1	D	257	SER
1	D	264	VAL
1	D	270	MET
1	D	271	THR
1	D	286	LYS
1	D	288	ILE
1	D	293	LEU
1	D	298	THR

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Mol	Chain	Res	Type
1	D	302	SER
1	D	304	ARG
1	D	305	LYS
1	D	307	ARG
1	D	309	GLU
1	D	310	LEU
1	D	311	ARG
1	D	318	SER
1	D	320	GLU
1	D	330	ILE
1	D	335	ILE
1	D	337	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	199	GLN
1	A	254	GLN
1	A	268	ASN
1	A	269	GLN
1	B	106	GLN
1	B	187	ASN
1	B	198	HIS
1	B	199	GLN
1	B	254	GLN
1	B	268	ASN
1	C	134	GLN
1	C	163	ASN
1	C	198	HIS
1	C	199	GLN
1	C	244	GLN
1	C	268	ASN
1	D	100	HIS
1	D	198	HIS
1	D	199	GLN
1	D	268	ASN
1	D	324	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	241/265 (90%)	-0.46	4 (1%) 69 64	32, 54, 111, 139	0
1	B	241/265 (90%)	-0.30	6 (2%) 58 52	35, 64, 120, 158	0
1	C	241/265 (90%)	-0.36	2 (0%) 82 80	32, 61, 113, 155	0
1	D	241/265 (90%)	-0.28	10 (4%) 41 36	38, 64, 123, 162	0
All	All	964/1060 (90%)	-0.35	22 (2%) 61 55	32, 61, 119, 162	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	PHE	3.9
1	D	128	PHE	3.9
1	B	235	GLY	3.7
1	C	128	PHE	3.5
1	A	128	PHE	3.4
1	D	84	GLY	3.4
1	D	235	GLY	3.2
1	A	231	VAL	3.1
1	A	235	GLY	3.0
1	D	233	PHE	2.8
1	D	286	LYS	2.8
1	C	235	GLY	2.8
1	B	130	THR	2.4
1	B	338	ALA	2.4
1	D	307	ARG	2.3
1	D	231	VAL	2.3
1	A	234	SER	2.2
1	D	234	SER	2.2
1	D	271	THR	2.1
1	D	310	LEU	2.1
1	B	310	LEU	2.0
1	B	84	GLY	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.