



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:43 PM UTC

PDB ID : 3LPX / pdb_00003lpx
Title : Crystal structure of GyrA
Authors : Jung, H.Y.; Heo, Y.S.
Deposited on : 2010-02-07
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

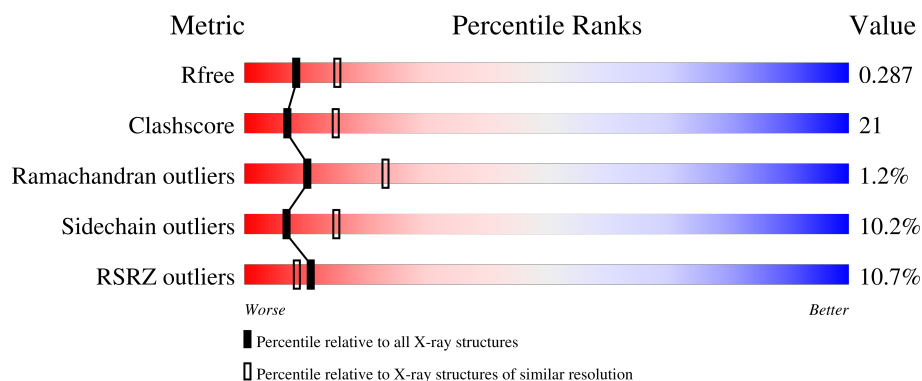
1 Overall quality at a glance

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	500	
1	B	500	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7331 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 DNA gyrase, A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3644	2296	643	687	18			
1	B	458	Total	C	N	O	S	0	0	0
			3608	2275	637	678	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	expression tag	UNP Q482G7
A	523	LEU	-	expression tag	UNP Q482G7
A	524	GLU	-	expression tag	UNP Q482G7
A	525	HIS	-	expression tag	UNP Q482G7
A	526	HIS	-	expression tag	UNP Q482G7
A	527	HIS	-	expression tag	UNP Q482G7
A	528	HIS	-	expression tag	UNP Q482G7
A	529	HIS	-	expression tag	UNP Q482G7
A	530	HIS	-	expression tag	UNP Q482G7
B	31	MET	-	expression tag	UNP Q482G7
B	523	LEU	-	expression tag	UNP Q482G7
B	524	GLU	-	expression tag	UNP Q482G7
B	525	HIS	-	expression tag	UNP Q482G7
B	526	HIS	-	expression tag	UNP Q482G7
B	527	HIS	-	expression tag	UNP Q482G7
B	528	HIS	-	expression tag	UNP Q482G7
B	529	HIS	-	expression tag	UNP Q482G7
B	530	HIS	-	expression tag	UNP Q482G7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		

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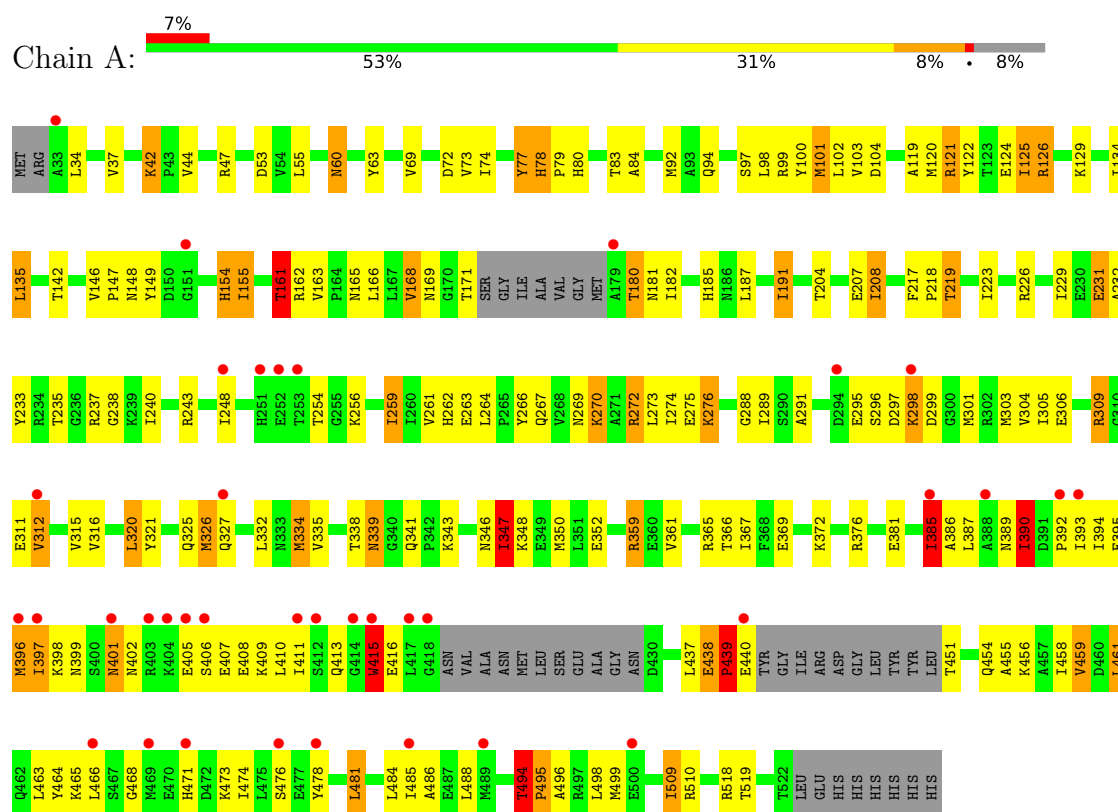
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	35	Total	O	0	0
			35	35		

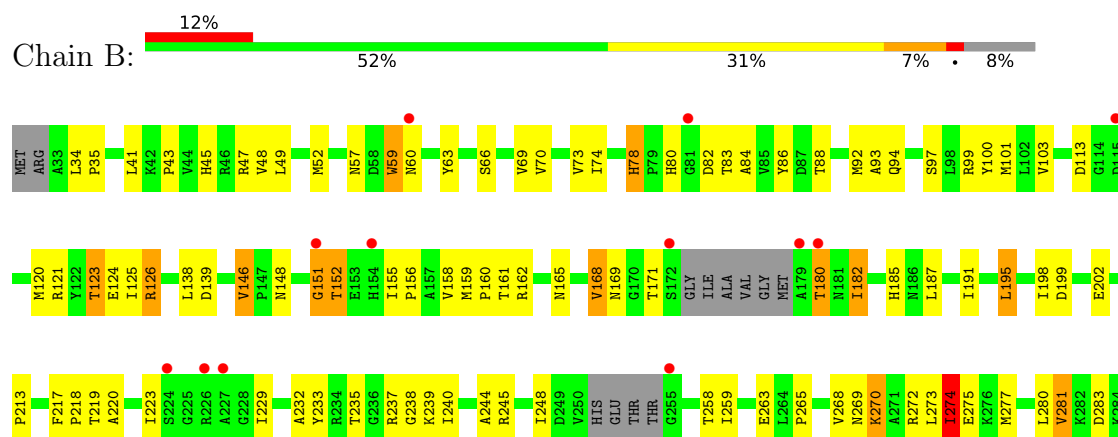
3 Residue-property plots

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: DNA gyrase, A subunit



• Molecule 1: DNA gyrase, A subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.98Å 101.56Å 141.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.29 – 2.60 41.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.29-2.60) 97.1 (41.29-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.262 , 0.287 0.262 , 0.287	Depositor DCC
R_{free} test set	2169 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7331	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.66	0/3700	1.29	44/4995 (0.9%)
1	B	0.69	0/3662	1.23	45/4941 (0.9%)
All	All	0.67	0/7362	1.26	89/9936 (0.9%)

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ILE	N-CA-C	-18.09	94.49	111.67
1	A	80	HIS	N-CA-C	11.12	127.72	112.93
1	A	298	LYS	N-CA-C	-10.79	99.52	112.89
1	B	390	ILE	N-CA-C	9.97	119.81	110.74
1	A	415	TRP	N-CA-C	9.42	125.29	110.32
1	A	326	MET	N-CA-C	-8.62	102.03	112.54
1	A	437	LEU	N-CA-C	8.20	121.60	108.41
1	B	470	GLU	N-CA-C	-8.06	102.08	112.23
1	B	340	GLY	N-CA-C	-7.41	98.76	112.62
1	A	476	SER	N-CA-C	-7.34	102.24	112.45
1	B	456	LYS	N-CA-C	-7.33	103.00	112.23
1	B	161	THR	N-CA-C	7.25	121.17	110.30
1	B	326	MET	N-CA-C	-7.20	103.47	111.82
1	A	438	GLU	CA-C-N	7.18	128.82	119.84
1	A	438	GLU	C-N-CA	7.18	128.82	119.84
1	A	390	ILE	N-CA-C	6.99	121.95	111.89
1	A	162	ARG	N-CA-C	-6.83	104.69	113.16
1	B	312	VAL	N-CA-C	6.79	123.47	109.34
1	B	346	ASN	N-CA-C	-6.75	100.53	110.52
1	A	83	THR	N-CA-C	-6.69	103.06	113.02
1	B	152	THR	N-CA-C	6.53	124.70	110.80
1	B	345	PHE	O-C-N	-6.51	114.73	123.19
1	B	83	THR	N-CA-C	-6.45	103.84	112.94
1	A	494	THR	N-CA-C	6.37	121.08	108.59
1	A	161	THR	N-CA-C	6.34	119.55	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ASN	N-CA-C	-6.34	101.40	110.59
1	B	310	GLY	N-CA-C	-6.30	100.24	110.95
1	B	387	LEU	N-CA-C	-6.18	102.20	110.55
1	B	347	ILE	CB-CA-C	-6.17	103.81	112.14
1	B	202	GLU	N-CA-C	-6.08	105.70	112.57
1	B	60	ASN	N-CA-C	6.06	119.14	111.69
1	A	84	ALA	N-CA-C	-6.02	104.41	110.97
1	B	397	ILE	N-CA-C	-6.01	104.48	110.62
1	B	182	ILE	CA-C-N	5.99	126.55	120.38
1	B	182	ILE	C-N-CA	5.99	126.55	120.38
1	B	386	ALA	N-CA-C	-5.96	104.17	112.45
1	B	406	SER	N-CA-C	-5.95	104.38	111.69
1	A	385	ILE	N-CA-C	-5.89	103.54	111.44
1	A	341	GLN	N-CA-C	5.89	119.79	109.48
1	A	161	THR	CB-CA-C	-5.88	100.73	109.90
1	B	244	ALA	N-CA-C	-5.87	102.62	110.55
1	B	146	VAL	CA-C-N	-5.85	113.95	119.85
1	B	146	VAL	C-N-CA	-5.85	113.95	119.85
1	A	334	MET	N-CA-C	5.80	118.83	107.57
1	B	165	ASN	N-CA-C	5.80	118.38	111.71
1	A	496	ALA	N-CA-C	5.77	117.64	111.36
1	A	122	TYR	N-CA-C	5.75	119.88	112.41
1	A	74	ILE	CB-CA-C	-5.74	104.62	111.97
1	B	151	GLY	N-CA-C	-5.74	99.59	113.18
1	B	287	GLU	N-CA-C	5.72	122.98	110.80
1	B	390	ILE	CB-CA-C	-5.71	104.41	111.94
1	B	416	GLU	N-CA-C	-5.70	101.76	110.14
1	A	77	TYR	N-CA-C	5.66	122.86	110.80
1	A	401	ASN	N-CA-C	5.66	119.27	112.93
1	A	413	GLN	N-CA-C	-5.63	101.69	110.42
1	A	312	VAL	N-CA-C	5.62	116.50	107.73
1	A	78	HIS	CA-C-N	5.58	126.82	119.84
1	A	78	HIS	C-N-CA	5.58	126.82	119.84
1	B	286	LEU	CA-C-N	5.58	132.20	121.54
1	B	286	LEU	C-N-CA	5.58	132.20	121.54
1	B	341	GLN	CB-CA-C	-5.58	99.17	110.17
1	B	414	GLY	N-CA-C	-5.56	100.01	113.18
1	B	288	GLY	N-CA-C	5.54	126.31	113.18
1	B	274	ILE	CB-CA-C	-5.54	104.67	112.14
1	A	191	ILE	N-CA-C	-5.52	105.14	110.72
1	A	295	GLU	N-CA-C	-5.52	104.79	112.30
1	A	226	ARG	N-CA-C	5.52	122.55	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ILE	N-CA-C	-5.48	100.52	108.36
1	A	60	ASN	CB-CA-C	-5.47	100.70	110.70
1	A	272	ARG	N-CA-C	-5.38	105.49	111.36
1	B	395	GLU	N-CA-C	5.38	118.64	111.75
1	B	308	LYS	N-CA-C	5.29	122.06	110.80
1	B	341	GLN	N-CA-C	5.29	121.49	109.81
1	A	304	VAL	N-CA-C	5.28	115.46	107.75
1	A	396	MET	CB-CA-C	-5.26	99.95	110.42
1	B	138	LEU	N-CA-C	-5.26	106.13	112.54
1	A	165	ASN	N-CA-C	5.25	117.01	111.28
1	A	42	LYS	N-CA-C	-5.25	103.53	110.40
1	B	235	THR	N-CA-C	5.24	120.15	113.55
1	A	399	ASN	N-CA-C	5.21	119.20	113.21
1	A	208	ILE	CB-CA-C	-5.19	105.13	112.14
1	B	195	LEU	N-CA-C	-5.16	105.55	111.07
1	A	367	ILE	CB-CA-C	-5.15	105.38	111.97
1	B	299	ASP	N-CA-C	5.13	119.18	113.02
1	A	149	TYR	N-CA-C	5.12	118.30	111.75
1	A	347	ILE	N-CA-C	5.08	117.40	111.05
1	B	78	HIS	CA-C-N	5.05	126.15	119.84
1	B	78	HIS	C-N-CA	5.05	126.15	119.84
1	A	406	SER	N-CA-C	-5.02	105.50	110.97

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	3644	0	3700	150	0
1	B	3608	0	3671	162	0
2	A	44	0	0	3	0
2	B	35	0	0	0	0
All	All	7331	0	7371	305	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 21.

All (305) 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:308:LYS:O	1:B:309:ARG:HG3	1.22	1.36
1:A:321:TYR:O	1:A:327:GLN:HG2	1.61	1.00
1:B:308:LYS:O	1:B:309:ARG:CG	2.12	0.96
1:A:395:GLU:HG3	1:A:398:LYS:HB2	1.51	0.93
1:A:459:VAL:HG13	1:B:464:TYR:HB3	1.48	0.92
1:A:291:ALA:HB3	1:A:306:GLU:HG3	1.51	0.92
1:B:289:ILE:HD11	1:B:316:VAL:HG11	1.54	0.90
1:B:155:ILE:HG13	1:B:156:PRO:HD2	1.52	0.89
1:A:101:MET:HE3	1:A:101:MET:H	1.36	0.88
1:A:243:ARG:NH1	1:A:327:GLN:HB2	1.92	0.85
1:B:182:ILE:HD11	1:B:334:MET:HA	1.59	0.84
1:A:461:LEU:HD22	1:A:465:LYS:HG3	1.58	0.83
1:B:100:TYR:H	1:B:169:ASN:HD21	1.26	0.83
1:A:297:ASP:HB3	1:A:299:ASP:H	1.44	0.82
1:A:134:ILE:HG23	1:A:161:THR:HG23	1.61	0.82
1:A:395:GLU:C	1:A:397:ILE:H	1.86	0.80
1:B:410:LEU:HA	1:B:415:TRP:HH2	1.46	0.80
1:A:395:GLU:HG2	1:A:396:MET:H	1.44	0.80
1:A:248:ILE:O	1:A:248:ILE:HG13	1.80	0.79
1:B:287:GLU:HG2	1:B:288:GLY:H	1.48	0.78
1:A:191:ILE:HD11	1:A:509:ILE:HD11	1.65	0.78
1:A:180:THR:HG23	1:A:335:VAL:H	1.48	0.77
1:B:388:ALA:H	1:B:390:ILE:HD11	1.49	0.77
1:A:408:GLU:HA	1:A:411:ILE:HG12	1.64	0.77
1:A:464:TYR:HB3	1:B:459:VAL:HG13	1.68	0.76
1:A:269:ASN:HB3	1:A:272:ARG:HE	1.51	0.76
1:B:191:ILE:HD11	1:B:509:ILE:HD11	1.68	0.76
1:B:269:ASN:ND2	1:B:272:ARG:HE	1.84	0.75
1:A:223:ILE:HD12	1:A:240:ILE:HD12	1.69	0.75
1:A:261:VAL:HG11	1:A:326:MET:HE1	1.68	0.74
1:A:217:PHE:HE2	1:A:223:ILE:HD11	1.52	0.74
1:A:262:HIS:C	1:A:301:MET:HE2	2.12	0.74
1:A:276:LYS:HE3	1:A:325:GLN:HG3	1.70	0.73
1:B:516:GLU:CD	1:B:516:GLU:H	1.94	0.72
1:B:113:ASP:OD1	1:B:270:LYS:HB3	1.90	0.72
1:B:347:ILE:HA	1:B:350:MET:HE3	1.74	0.70
1:B:410:LEU:HA	1:B:415:TRP:CH2	2.27	0.70
1:A:219:THR:HG21	1:A:266:TYR:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HB	1:A:303:MET:HB2	1.74	0.69
1:B:48:VAL:HG12	1:B:52:MET:HE2	1.74	0.69
1:B:383:LEU:HD23	1:B:458:ILE:HD13	1.76	0.68
1:B:103:VAL:HG11	1:B:125:ILE:HD12	1.74	0.68
1:B:407:GLU:HA	1:B:410:LEU:HD12	1.74	0.68
1:B:491:ILE:HG22	1:B:498:LEU:HD12	1.76	0.67
1:A:204:THR:HG23	1:A:207:GLU:H	1.59	0.67
1:A:410:LEU:HA	1:A:415:TRP:HZ3	1.60	0.67
1:B:180:THR:HG23	1:B:335:VAL:HB	1.76	0.67
1:A:464:TYR:HB3	1:B:459:VAL:CG1	2.26	0.66
1:B:217:PHE:HE2	1:B:223:ILE:HD11	1.61	0.66
1:A:273:LEU:HA	1:A:276:LYS:HE2	1.78	0.66
1:A:389:ASN:O	1:A:393:ILE:HG12	1.96	0.65
1:B:334:MET:SD	1:B:350:MET:HE1	2.36	0.65
1:B:481:LEU:O	1:B:485:ILE:HG23	1.97	0.65
1:B:43:PRO:O	1:B:47:ARG:HG3	1.97	0.65
1:B:289:ILE:HD11	1:B:316:VAL:CG1	2.26	0.64
1:A:218:PRO:HA	1:A:518:ARG:HH11	1.63	0.64
1:B:387:LEU:HA	1:B:390:ILE:HG13	1.80	0.63
1:B:269:ASN:HD22	1:B:272:ARG:HE	1.46	0.62
1:A:395:GLU:C	1:A:397:ILE:N	2.56	0.62
1:B:396:MET:SD	1:B:409:LYS:HB3	2.39	0.62
1:B:402:ASN:ND2	1:B:404:LYS:HB2	2.14	0.62
1:A:396:MET:HE2	1:A:409:LYS:HB3	1.82	0.61
1:A:44:VAL:HG23	2:A:14:HOH:O	2.00	0.61
1:B:233:TYR:HB3	1:B:347:ILE:CG1	2.30	0.61
1:A:259:ILE:HG12	1:A:305:ILE:HD13	1.82	0.61
1:A:94:GLN:HB2	1:A:97:SER:HB2	1.83	0.61
1:A:410:LEU:HA	1:A:415:TRP:CZ3	2.36	0.61
1:B:182:ILE:HG13	1:B:334:MET:HG2	1.81	0.61
1:B:338:THR:O	1:B:339:ASN:HB2	2.00	0.61
1:A:120:MET:HG2	1:A:121:ARG:HH12	1.65	0.60
1:B:454:GLN:O	1:B:458:ILE:HG12	2.00	0.60
1:A:161:THR:HG22	1:A:163:VAL:H	1.66	0.60
1:A:264:LEU:HG	1:A:301:MET:HE1	1.84	0.60
1:A:100:TYR:H	1:A:169:ASN:HD21	1.50	0.60
1:B:265:PRO:O	1:B:268:VAL:HG22	2.02	0.60
1:B:390:ILE:HD12	1:B:390:ILE:H	1.66	0.60
1:A:389:ASN:O	1:A:392:PRO:HD2	2.02	0.59
1:A:204:THR:HG22	1:A:207:GLU:OE1	2.03	0.59
1:A:219:THR:HG21	1:A:266:TYR:CA	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLU:O	1:B:398:LYS:HB2	2.01	0.59
1:B:475:LEU:O	1:B:479:LYS:HG3	2.04	0.58
1:A:288:GLY:HA2	1:A:311:GLU:HG3	1.84	0.58
1:A:390:ILE:HD12	1:A:466:LEU:HD23	1.84	0.58
1:B:182:ILE:CD1	1:B:334:MET:HA	2.32	0.58
1:B:270:LYS:HD3	1:B:301:MET:HE2	1.84	0.58
1:B:277:MET:O	1:B:281:VAL:HG12	2.04	0.58
1:A:465:LYS:HE3	2:A:547:HOH:O	2.03	0.58
1:B:155:ILE:HG13	1:B:156:PRO:CD	2.28	0.58
1:A:359:ARG:HD3	1:A:499:MET:SD	2.44	0.58
1:A:92:MET:HE2	1:A:102:LEU:HD12	1.86	0.57
1:B:316:VAL:O	1:B:320:LEU:HB2	2.04	0.57
1:A:401:ASN:O	1:B:469:MET:HG2	2.05	0.57
1:B:365:ARG:O	1:B:369:GLU:HG2	2.05	0.57
1:A:396:MET:HE1	1:A:415:TRP:HH2	1.70	0.57
1:A:365:ARG:O	1:A:369:GLU:HG2	2.05	0.56
1:A:182:ILE:HG12	1:A:334:MET:HG2	1.88	0.56
1:B:100:TYR:CD2	1:B:168:VAL:HG13	2.40	0.56
1:B:410:LEU:O	1:B:415:TRP:HZ3	1.87	0.56
1:A:309:ARG:HH11	1:A:309:ARG:HG2	1.70	0.56
1:B:474:ILE:HD13	1:B:475:LEU:N	2.20	0.56
1:A:146:VAL:HB	1:A:147:PRO:HD2	1.87	0.56
1:B:198:ILE:HD12	1:B:499:MET:CE	2.36	0.56
1:B:387:LEU:HD13	1:B:471:HIS:ND1	2.20	0.56
1:B:485:ILE:HD12	1:B:489:MET:HE2	1.88	0.56
1:B:82:ASP:HB3	1:B:84:ALA:H	1.71	0.55
1:B:280:LEU:HB3	1:B:286:LEU:HB2	1.88	0.55
1:A:63:TYR:HB3	1:A:124:GLU:HB3	1.88	0.55
1:A:466:LEU:H	1:A:466:LEU:HD12	1.72	0.55
1:B:180:THR:HG22	1:B:182:ILE:CD1	2.36	0.55
1:B:474:ILE:HD13	1:B:475:LEU:H	1.72	0.55
1:A:390:ILE:HD12	1:B:398:LYS:HE2	1.89	0.55
1:B:180:THR:HG21	1:B:335:VAL:O	2.07	0.55
1:A:264:LEU:HD11	1:A:270:LYS:HG3	1.89	0.55
1:A:37:VAL:HA	1:A:166:LEU:HD22	1.90	0.55
1:B:389:ASN:O	1:B:393:ILE:HG12	2.07	0.54
1:A:338:THR:HG23	1:A:339:ASN:H	1.71	0.54
1:B:49:LEU:HD23	1:B:52:MET:HE3	1.90	0.54
1:B:233:TYR:CG	1:B:347:ILE:HG12	2.42	0.54
1:B:430:ASP:O	1:B:433:ARG:HG2	2.07	0.54
1:A:134:ILE:HA	1:A:161:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:THR:O	1:B:338:THR:HG23	2.08	0.53
1:A:218:PRO:HA	1:A:518:ARG:NH1	2.23	0.53
1:A:466:LEU:HD12	1:A:466:LEU:N	2.24	0.53
1:A:187:LEU:O	1:A:191:ILE:HG12	2.09	0.53
1:A:387:LEU:HB3	1:A:471:HIS:CE1	2.43	0.53
1:A:55:LEU:HD11	1:A:72:ASP:OD2	2.08	0.52
1:A:229:ILE:HD13	1:A:240:ILE:HG21	1.92	0.52
1:B:245:ARG:HB3	1:B:263:GLU:CG	2.39	0.52
1:A:458:ILE:O	1:A:461:LEU:HB2	2.09	0.52
1:A:407:GLU:OE2	1:A:456:LYS:HG2	2.10	0.52
1:A:185:HIS:HE1	1:A:233:TYR:OH	1.93	0.52
1:B:340:GLY:O	1:B:341:GLN:HB2	2.11	0.51
1:B:66:SER:OG	1:B:123:THR:HG23	2.10	0.51
1:B:103:VAL:CG1	1:B:125:ILE:HD12	2.38	0.51
1:A:312:VAL:HG11	1:A:315:VAL:HG23	1.92	0.51
1:A:99:ARG:HA	1:A:218:PRO:HB3	1.93	0.51
1:A:142:THR:HB	1:A:361:VAL:HG13	1.91	0.51
1:B:484:LEU:HD22	1:B:488:LEU:HG	1.92	0.51
1:B:94:GLN:HB2	1:B:97:SER:HB2	1.93	0.50
1:B:69:VAL:O	1:B:73:VAL:HG23	2.10	0.50
1:B:63:TYR:CE1	1:B:126:ARG:HD2	2.46	0.50
1:B:80:HIS:C	1:B:82:ASP:H	2.18	0.50
1:B:346:ASN:ND2	1:B:349:GLU:HG3	2.27	0.50
1:B:378:HIS:CE1	1:B:454:GLN:HG3	2.47	0.50
1:B:248:ILE:HG12	1:B:259:ILE:HD13	1.92	0.50
1:B:404:LYS:HE3	1:B:404:LYS:N	2.26	0.50
1:B:182:ILE:HD12	1:B:182:ILE:N	2.27	0.50
1:A:100:TYR:CD2	1:A:168:VAL:HG13	2.47	0.49
1:B:237:ARG:HA	1:B:332:LEU:O	2.12	0.49
1:A:119:ALA:HB1	1:A:121:ARG:CZ	2.42	0.49
1:B:233:TYR:HB3	1:B:347:ILE:HD11	1.94	0.49
1:A:393:ILE:O	1:A:397:ILE:HD13	2.13	0.49
1:A:231:GLU:O	1:A:235:THR:HB	2.13	0.49
1:B:74:ILE:HA	1:B:78:HIS:O	2.13	0.49
1:B:245:ARG:HB3	1:B:263:GLU:HG2	1.94	0.49
1:A:261:VAL:HG12	1:A:301:MET:CE	2.43	0.48
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.78	0.48
1:A:101:MET:H	1:A:101:MET:CE	2.19	0.48
1:B:63:TYR:HB3	1:B:124:GLU:HB3	1.95	0.48
1:B:223:ILE:HD12	1:B:240:ILE:HD12	1.95	0.48
1:A:134:ILE:CG2	1:A:161:THR:HG23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HG	1:A:301:MET:CE	2.44	0.48
1:A:366:THR:HG23	1:A:488:LEU:HD22	1.96	0.48
1:A:223:ILE:HG12	1:A:519:THR:HG21	1.95	0.48
1:A:264:LEU:HG	1:A:301:MET:SD	2.54	0.48
1:A:395:GLU:O	1:A:396:MET:HB2	2.13	0.48
1:B:380:LEU:HD23	1:B:383:LEU:HD12	1.96	0.48
1:B:274:ILE:HG22	1:B:292:LEU:HD13	1.96	0.48
1:A:182:ILE:HD13	1:A:350:MET:HE1	1.96	0.47
1:A:219:THR:HG21	1:A:266:TYR:N	2.30	0.47
1:B:171:THR:HG22	1:B:182:ILE:HB	1.95	0.47
1:A:389:ASN:O	1:A:389:ASN:OD1	2.32	0.47
1:A:455:ALA:O	1:A:459:VAL:HB	2.15	0.47
1:A:464:TYR:CB	1:B:459:VAL:HG13	2.42	0.47
1:B:92:MET:HE3	1:B:103:VAL:CG2	2.45	0.47
1:B:396:MET:SD	1:B:409:LYS:O	2.72	0.47
1:B:413:GLN:HB2	1:B:415:TRP:CZ3	2.50	0.47
1:B:461:LEU:HD11	1:B:465:LYS:HB2	1.97	0.47
1:B:485:ILE:CD1	1:B:489:MET:HE2	2.44	0.47
1:B:35:PRO:HG3	1:B:171:THR:HG21	1.97	0.47
1:A:297:ASP:HB3	1:A:299:ASP:N	2.22	0.47
1:A:134:ILE:HG12	1:A:161:THR:CG2	2.45	0.47
1:A:509:ILE:HG13	1:A:510:ARG:N	2.29	0.47
1:B:125:ILE:CG2	1:B:126:ARG:N	2.78	0.47
1:A:270:LYS:HE2	1:A:296:SER:OG	2.15	0.46
1:A:338:THR:HG23	1:A:339:ASN:N	2.30	0.46
1:A:390:ILE:O	1:A:394:ILE:HG12	2.15	0.46
1:A:395:GLU:HG2	1:A:396:MET:N	2.23	0.46
1:A:103:VAL:HG13	1:A:125:ILE:HG13	1.97	0.46
1:A:274:ILE:HG13	1:A:303:MET:HE3	1.98	0.46
1:A:454:GLN:O	1:A:458:ILE:HD13	2.16	0.46
1:B:180:THR:CG2	1:B:335:VAL:O	2.64	0.46
1:A:163:VAL:HG22	1:A:509:ILE:HD13	1.97	0.46
1:A:335:VAL:HA	1:A:343:LYS:O	2.15	0.46
1:B:99:ARG:HA	1:B:218:PRO:HB3	1.98	0.46
1:B:113:ASP:OD1	1:B:270:LYS:NZ	2.48	0.46
1:B:237:ARG:HE	1:B:333:ASN:ND2	2.14	0.46
1:B:413:GLN:HB2	1:B:415:TRP:CH2	2.51	0.46
1:B:501:VAL:O	1:B:505:GLU:HG3	2.16	0.46
1:B:100:TYR:H	1:B:169:ASN:ND2	2.05	0.46
1:B:185:HIS:HE1	1:B:233:TYR:OH	1.98	0.46
1:A:261:VAL:HG12	1:A:301:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:CE1	1:A:126:ARG:HD2	2.50	0.46
1:B:88:THR:O	1:B:92:MET:HG3	2.15	0.46
1:B:387:LEU:HA	1:B:390:ILE:CG1	2.44	0.46
1:A:235:THR:HG22	1:A:237:ARG:H	1.81	0.46
1:B:48:VAL:CG1	1:B:52:MET:HE2	2.44	0.46
1:B:217:PHE:CE2	1:B:223:ILE:HD11	2.47	0.46
1:A:312:VAL:CG1	1:A:315:VAL:HG23	2.46	0.45
1:B:59:TRP:HA	1:B:126:ARG:HG3	1.97	0.45
1:B:407:GLU:O	1:B:410:LEU:HB2	2.16	0.45
1:B:265:PRO:HD2	1:B:268:VAL:HG21	1.97	0.45
1:A:171:THR:HG22	1:A:182:ILE:HB	1.97	0.45
1:B:70:VAL:HG11	1:B:120:MET:HE1	1.97	0.45
1:B:461:LEU:CD1	1:B:465:LYS:HB2	2.46	0.45
1:A:451:THR:HB	2:A:556:HOH:O	2.17	0.45
1:B:233:TYR:HB3	1:B:347:ILE:HG12	1.97	0.45
1:A:104:ASP:OD2	1:A:126:ARG:HD3	2.16	0.45
1:A:208:ILE:HD13	1:A:347:ILE:HG23	1.98	0.45
1:B:386:ALA:CB	1:B:458:ILE:HD12	2.47	0.45
1:A:439:PRO:HB2	1:A:440:GLU:OE2	2.16	0.44
1:B:198:ILE:HD11	1:B:355:VAL:CG1	2.46	0.44
1:B:402:ASN:ND2	1:B:404:LYS:H	2.14	0.44
1:A:395:GLU:O	1:A:397:ILE:N	2.50	0.44
1:B:324:THR:OG1	1:B:326:MET:HG2	2.17	0.44
1:A:407:GLU:HA	1:A:410:LEU:HD13	1.98	0.44
1:B:335:VAL:HA	1:B:343:LYS:O	2.18	0.44
1:B:346:ASN:CG	1:B:349:GLU:HG3	2.43	0.44
1:A:376:ARG:HG2	1:A:481:LEU:HD21	2.00	0.44
1:A:395:GLU:CG	1:A:396:MET:H	2.22	0.44
1:B:233:TYR:CB	1:B:347:ILE:CG1	2.96	0.44
1:A:395:GLU:O	1:A:396:MET:CB	2.65	0.44
1:B:195:LEU:HD23	1:B:195:LEU:HA	1.86	0.44
1:A:121:ARG:H	1:A:121:ARG:HG2	1.64	0.44
1:A:348:LYS:HG2	1:A:352:GLU:OE2	2.17	0.44
1:B:93:ALA:O	1:B:101:MET:HE3	2.18	0.43
1:B:310:GLY:C	1:B:312:VAL:H	2.25	0.43
1:B:402:ASN:HD22	1:B:404:LYS:HB2	1.82	0.43
1:A:47:ARG:NH1	1:A:78:HIS:HD2	2.16	0.43
1:B:162:ARG:HG3	1:B:358:ARG:NH2	2.33	0.43
1:B:233:TYR:CB	1:B:347:ILE:HG12	2.48	0.43
1:A:385:ILE:HD13	1:A:386:ALA:N	2.34	0.43
1:B:34:LEU:HD12	1:B:34:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PRO:O	1:B:229:ILE:HG21	2.18	0.43
1:A:289:ILE:HD11	1:A:316:VAL:HG13	2.01	0.43
1:B:219:THR:O	1:B:220:ALA:HB3	2.18	0.43
1:B:233:TYR:HB3	1:B:347:ILE:CD1	2.49	0.43
1:A:325:GLN:C	1:A:327:GLN:N	2.73	0.43
1:A:402:ASN:OD1	1:A:405:GLU:HB3	2.19	0.43
1:B:168:VAL:HG21	1:B:187:LEU:HD13	2.01	0.43
1:A:69:VAL:O	1:A:73:VAL:HG23	2.19	0.43
1:A:273:LEU:HD21	1:A:326:MET:HE3	2.00	0.43
1:B:287:GLU:CG	1:B:288:GLY:H	2.17	0.43
1:B:324:THR:C	1:B:326:MET:H	2.27	0.43
1:B:347:ILE:H	1:B:347:ILE:HG13	1.66	0.43
1:A:381:GLU:HG3	1:A:478:TYR:CZ	2.54	0.42
1:B:93:ALA:C	1:B:101:MET:HE3	2.44	0.42
1:B:391:ASP:HB2	1:B:392:PRO:HD3	2.01	0.42
1:A:464:TYR:HA	1:B:397:ILE:HG21	2.00	0.42
1:B:92:MET:HE3	1:B:103:VAL:HG23	2.00	0.42
1:B:159:MET:HA	1:B:160:PRO:HD3	1.77	0.42
1:B:288:GLY:O	1:B:289:ILE:HD13	2.19	0.42
1:A:154:HIS:C	1:A:155:ILE:HD13	2.45	0.42
1:A:494:THR:O	1:A:495:PRO:C	2.62	0.42
1:B:270:LYS:O	1:B:274:ILE:HG12	2.20	0.42
1:B:283:ASP:HB2	1:B:285:ARG:HG3	2.01	0.42
1:A:485:ILE:HG13	1:A:486:ALA:N	2.34	0.42
1:B:66:SER:OG	1:B:123:THR:CG2	2.67	0.42
1:B:393:ILE:O	1:B:394:ILE:C	2.62	0.42
1:B:41:LEU:HD22	1:B:45:HIS:HB3	2.01	0.42
1:B:148:ASN:OD1	1:B:151:GLY:O	2.38	0.42
1:B:312:VAL:HG23	1:B:312:VAL:O	2.18	0.42
1:A:229:ILE:CD1	1:A:240:ILE:HG21	2.50	0.41
1:B:198:ILE:HD11	1:B:355:VAL:HG11	2.01	0.41
1:A:99:ARG:HG3	1:A:100:TYR:CE2	2.55	0.41
1:A:267:GLN:HE21	1:A:267:GLN:HB2	1.61	0.41
1:A:77:TYR:CD1	1:A:155:ILE:HD12	2.56	0.41
1:B:390:ILE:HG22	1:B:394:ILE:CD1	2.50	0.41
1:A:148:ASN:HB3	1:A:155:ILE:HD11	2.03	0.41
1:A:347:ILE:O	1:A:347:ILE:HG13	2.21	0.41
1:A:263:GLU:N	1:A:301:MET:HE2	2.34	0.41
1:A:320:LEU:HD12	1:A:320:LEU:HA	1.85	0.41
1:B:125:ILE:HG22	1:B:126:ARG:N	2.35	0.41
1:A:134:ILE:HG12	1:A:161:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLU:HA	1:A:398:LYS:HG3	2.02	0.41
1:A:92:MET:HA	1:A:98:LEU:HD22	2.01	0.41
1:A:180:THR:HG22	1:A:181:ASN:H	1.85	0.41
1:B:232:ALA:HB2	1:B:238:GLY:HA3	2.01	0.41
1:B:273:LEU:HD23	1:B:303:MET:HE1	2.01	0.41
1:B:292:LEU:HD12	1:B:292:LEU:O	2.20	0.41
1:B:409:LYS:HD3	1:B:412:SER:OG	2.21	0.41
1:B:410:LEU:HD23	1:B:415:TRP:CH2	2.56	0.41
1:A:53:ASP:HB2	1:A:135:LEU:HD12	2.02	0.41
1:A:254:THR:C	1:A:256:LYS:H	2.29	0.41
1:A:389:ASN:HD21	1:A:415:TRP:HD1	1.69	0.40
1:A:438:GLU:O	1:A:440:GLU:N	2.54	0.40
1:B:86:TYR:OH	1:B:123:THR:HG21	2.22	0.40
1:B:406:SER:O	1:B:410:LEU:HG	2.21	0.40
1:B:484:LEU:HD22	1:B:484:LEU:O	2.22	0.40
1:A:237:ARG:HA	1:A:332:LEU:O	2.22	0.40
1:B:191:ILE:HG21	1:B:510:ARG:HB2	2.03	0.40
1:A:180:THR:CG2	1:A:335:VAL:H	2.24	0.40
1:A:232:ALA:HB2	1:A:238:GLY:HA3	2.03	0.40
1:B:259:ILE:HB	1:B:305:ILE:HG23	2.03	0.40
1:A:180:THR:HG23	1:A:335:VAL:N	2.27	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	454/500 (91%)	430 (95%)	21 (5%)	3 (1%)	18	38
1	B	448/500 (90%)	410 (92%)	30 (7%)	8 (2%)	6	14
All	All	902/1000 (90%)	840 (93%)	51 (6%)	11 (1%)	10	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	PRO
1	B	152	THR
1	B	287	GLU
1	B	309	ARG
1	B	312	VAL
1	B	389	ASN
1	B	288	GLY
1	B	399	ASN
1	B	341	GLN
1	A	79	PRO
1	A	468	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/424 (93%)	351 (89%)	43 (11%)	6	13
1	B	390/424 (92%)	353 (90%)	37 (10%)	8	18
All	All	784/848 (92%)	704 (90%)	80 (10%)	7	15

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	42	LYS
1	A	60	ASN
1	A	101	MET
1	A	121	ARG
1	A	125	ILE
1	A	126	ARG
1	A	129	LYS
1	A	135	LEU
1	A	154	HIS
1	A	155	ILE
1	A	161	THR

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Mol	Chain	Res	Type
1	A	168	VAL
1	A	180	THR
1	A	219	THR
1	A	231	GLU
1	A	259	ILE
1	A	270	LYS
1	A	275	GLU
1	A	276	LYS
1	A	298	LYS
1	A	309	ARG
1	A	320	LEU
1	A	339	ASN
1	A	347	ILE
1	A	359	ARG
1	A	372	LYS
1	A	385	ILE
1	A	390	ILE
1	A	415	TRP
1	A	416	GLU
1	A	439	PRO
1	A	459	VAL
1	A	461	LEU
1	A	463	LEU
1	A	473	LYS
1	A	474	ILE
1	A	481	LEU
1	A	484	LEU
1	A	494	THR
1	A	495	PRO
1	A	498	LEU
1	A	509	ILE
1	B	57	ASN
1	B	59	TRP
1	B	121	ARG
1	B	123	THR
1	B	126	ARG
1	B	139	ASP
1	B	146	VAL
1	B	158	VAL
1	B	168	VAL
1	B	180	THR
1	B	199	ASP

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Mol	Chain	Res	Type
1	B	239	LYS
1	B	258	THR
1	B	270	LYS
1	B	274	ILE
1	B	275	GLU
1	B	281	VAL
1	B	286	LEU
1	B	298	LYS
1	B	305	ILE
1	B	318	ASN
1	B	332	LEU
1	B	347	ILE
1	B	356	LEU
1	B	390	ILE
1	B	396	MET
1	B	401	ASN
1	B	404	LYS
1	B	409	LYS
1	B	474	ILE
1	B	481	LEU
1	B	484	LEU
1	B	485	ILE
1	B	487	GLU
1	B	498	LEU
1	B	512	GLU
1	B	516	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	106	GLN
1	A	169	ASN
1	A	185	HIS
1	A	192	ASN
1	A	211	HIS
1	A	267	GLN
1	A	318	ASN
1	A	325	GLN
1	A	339	ASN
1	A	341	GLN
1	A	413	GLN

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Mol	Chain	Res	Type
1	A	471	HIS
1	B	57	ASN
1	B	78	HIS
1	B	106	GLN
1	B	169	ASN
1	B	181	ASN
1	B	185	HIS
1	B	211	HIS
1	B	262	HIS
1	B	319	ASN
1	B	333	ASN
1	B	341	GLN
1	B	357	HIS
1	B	389	ASN
1	B	401	ASN
1	B	402	ASN
1	B	413	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 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 ⓘ

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	462/500 (92%)	0.53	37 (8%)	18 14	32, 47, 70, 87	0
1	B	458/500 (91%)	0.66	61 (13%)	7 5	31, 47, 74, 87	0
All	All	920/1000 (92%)	0.59	98 (10%)	11 9	31, 47, 72, 87	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	ILE	5.6
1	B	393	ILE	5.0
1	B	418	GLY	4.5
1	B	401	ASN	4.4
1	A	418	GLY	4.3
1	B	411	ILE	4.2
1	A	397	ILE	4.0
1	A	393	ILE	3.9
1	B	415	TRP	3.9
1	B	310	GLY	3.7
1	B	469	MET	3.7
1	B	410	LEU	3.7
1	A	388	ALA	3.6
1	A	248	ILE	3.6
1	B	406	SER	3.5
1	B	389	ASN	3.5
1	B	463	LEU	3.4
1	B	398	LYS	3.3
1	B	385	ILE	3.3
1	B	451	THR	3.3
1	A	414	GLY	3.3
1	B	308	LYS	3.3
1	B	392	PRO	3.2
1	B	458	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	403	ARG	3.1
1	A	298	LYS	3.1
1	A	469	MET	3.1
1	A	385	ILE	3.1
1	B	412	SER	3.1
1	B	417	LEU	3.0
1	A	179	ALA	3.0
1	A	392	PRO	3.0
1	B	388	ALA	2.9
1	A	440	GLU	2.8
1	B	309	ARG	2.8
1	B	226	ARG	2.8
1	A	417	LEU	2.7
1	A	415	TRP	2.7
1	A	411	ILE	2.7
1	A	489	MET	2.7
1	B	387	LEU	2.7
1	B	179	ALA	2.7
1	A	476	SER	2.7
1	B	435	GLU	2.6
1	B	455	ALA	2.6
1	A	471	HIS	2.6
1	B	409	LYS	2.6
1	B	255	GLY	2.6
1	B	408	GLU	2.5
1	A	406	SER	2.5
1	B	172	SER	2.5
1	B	416	GLU	2.5
1	B	293	ARG	2.5
1	A	404	LYS	2.4
1	A	253	THR	2.4
1	B	396	MET	2.4
1	B	180	THR	2.4
1	A	478	TYR	2.4
1	B	439	PRO	2.4
1	A	412	SER	2.3
1	B	391	ASP	2.3
1	B	460	ASP	2.3
1	B	405	GLU	2.3
1	B	81	GLY	2.3
1	A	33	ALA	2.3
1	A	251	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	115	ASP	2.3
1	A	396	MET	2.3
1	A	294	ASP	2.3
1	B	470	GLU	2.2
1	A	401	ASN	2.2
1	B	60	ASN	2.2
1	A	312	VAL	2.2
1	B	403	ARG	2.2
1	A	466	LEU	2.2
1	B	298	LYS	2.2
1	B	414	GLY	2.2
1	A	252	GLU	2.2
1	B	474	ILE	2.2
1	A	405	GLU	2.1
1	A	500	GLU	2.1
1	B	468	GLY	2.1
1	B	227	ALA	2.1
1	B	287	GLU	2.1
1	B	479	LYS	2.1
1	B	288	GLY	2.1
1	A	485	ILE	2.1
1	B	430	ASP	2.1
1	B	400	SER	2.1
1	B	404	LYS	2.1
1	A	151	GLY	2.1
1	B	521	ILE	2.1
1	B	224	SER	2.0
1	B	522	THR	2.0
1	B	154	HIS	2.0
1	B	402	ASN	2.0
1	A	327	GLN	2.0
1	B	151	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.