



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:20 AM GMT

PDB ID : 3LPX
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

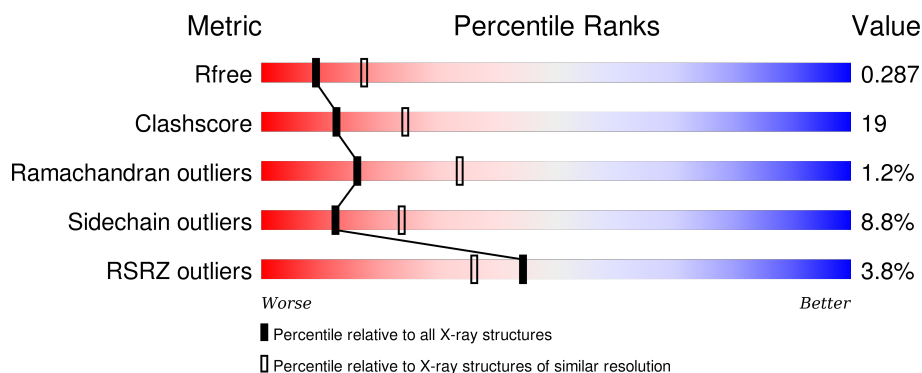
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	<div> <div>2%</div> <div>58%</div> <div>30%</div> <div>•</div> <div>8%</div> </div>
1	B	500	<div> <div>5%</div> <div>57%</div> <div>29%</div> <div>5%</div> <div>•</div> <div>8%</div> </div>

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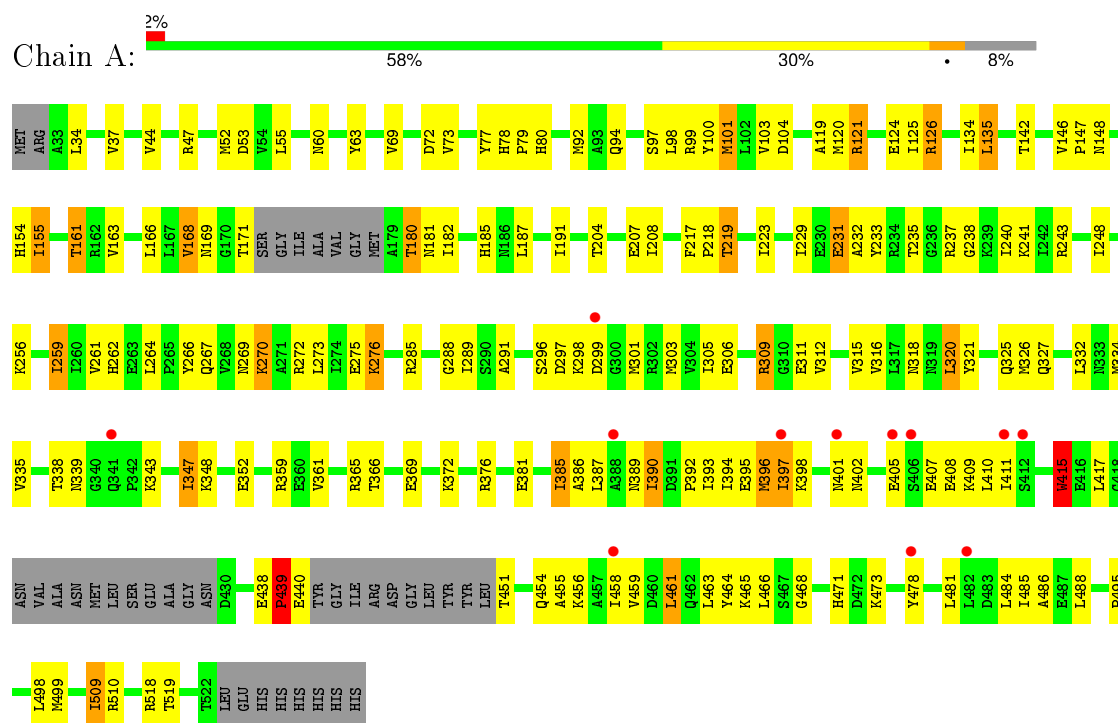
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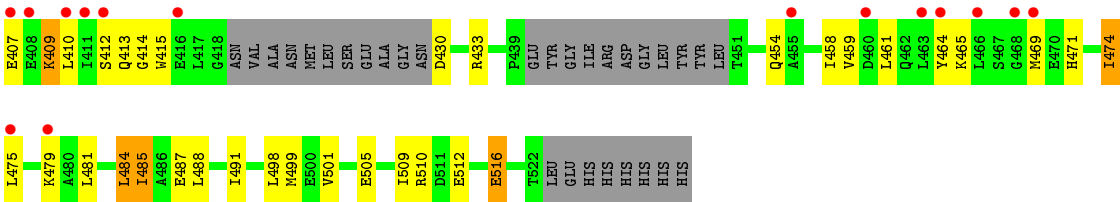
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	35	Total	O	0	0
			35	35		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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 41.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.29-2.60) 96.9 (41.28-2.60)	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 1.1	Depositor
R, R_{free}	0.262 , 0.287 0.262 , 0.287	Depositor DCC
R_{free} test set	2169 reflections (5.00%)	DCC
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 , 54.6	EDS
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43418 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/3700	0.84	5/4995 (0.1%)
1	B	0.55	0/3662	0.87	8/4941 (0.2%)
All	All	0.53	0/7362	0.85	13/9936 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	HIS	N-CA-C	6.19	127.72	111.00
1	A	397	ILE	N-CA-C	-6.12	94.49	111.00
1	B	340	GLY	N-CA-C	-5.73	98.76	113.10
1	A	417	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	341	GLN	CB-CA-C	-5.61	99.17	110.40
1	B	151	GLY	N-CA-C	-5.41	99.59	113.10
1	A	415	TRP	N-CA-C	5.29	125.29	111.00
1	B	288	GLY	N-CA-C	5.29	126.31	113.10
1	B	414	GLY	N-CA-C	-5.24	100.01	113.10
1	A	396	MET	CB-CA-C	-5.22	99.95	110.40
1	B	332	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	310	GLY	N-CA-C	-5.14	100.24	113.10
1	B	152	THR	N-CA-C	5.08	124.70	111.00

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	142	0
1	B	3608	0	3671	147	0
2	A	44	0	0	3	0
2	B	35	0	0	0	0
All	All	7331	0	7371	282	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 (282) 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: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: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:395:GLU:C	1:A:397:ILE:H	1.86	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:217:PHE:HE2	1:A:223:ILE:HD11	1.52	0.74
1:A:276:LYS:HE3	1:A:325:GLN:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ASP:OD1	1:B:270:LYS:HB3	1.90	0.72
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
1:A:261:VAL:HB	1:A:303:MET:HB2	1.74	0.69
1:B:516:GLU:H	1:B:516:GLU:CD	1.94	0.68
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:410:LEU:HA	1:A:415:TRP:HZ3	1.60	0.67
1:A:204:THR:HG23	1:A:207:GLU:H	1.59	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: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:A:261:VAL:HG11	1:A:326:MET:HE1	1.79	0.63
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:B:402:ASN:ND2	1:B:404:LYS:HB2	2.14	0.62
1:B:396:MET:SD	1:B:409:LYS:HB3	2.39	0.62
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:B:454:GLN:O	1:B:458:ILE:HG12	2.00	0.60
1:A:120:MET:HG2	1:A:121:ARG:HH12	1.65	0.60
1:A:161:THR:HG22	1:A:163:VAL:H	1.66	0.60
1:B:390:ILE:HD12	1:B:390:ILE:H	1.66	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: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:B:182:ILE:CD1	1:B:334:MET:HA	2.32	0.58
1:A:390:ILE:HD12	1:A:466:LEU:HD23	1.84	0.58
1:B:277:MET:O	1:B:281:VAL:HG12	2.04	0.58
1:B:155:ILE:HG13	1:B:156:PRO:CD	2.28	0.58
1:A:465:LYS:HE3	2:A:547:HOH:O	2.03	0.58
1:A:359:ARG:HD3	1:A:499:MET:SD	2.44	0.58
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:365:ARG:O	1:A:369:GLU:HG2	2.05	0.56
1:B:100:TYR:CD2	1:B:168:VAL:HG13	2.40	0.56
1:A:182:ILE:HG12	1:A:334:MET:HG2	1.88	0.56
1:A:101:MET:H	1:A:101:MET:CE	2.19	0.56
1:B:410:LEU:O	1:B:415:TRP:HZ3	1.87	0.56
1:A:262:HIS:C	1:A:301:MET:HE2	2.26	0.56
1:A:309:ARG:HG2	1:A:309:ARG:HH11	1.70	0.56
1:B:474:ILE:HD13	1:B:475:LEU:N	2.20	0.56
1:B:387:LEU:HD13	1:B:471:HIS:ND1	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:A:261:VAL:HG12	1:A:301:MET:HE3	1.88	0.55
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:B:180:THR:HG22	1:B:182:ILE:CD1	2.36	0.55
1:A:466:LEU:HD12	1:A:466:LEU:H	1.72	0.55
1:B:474:ILE:HD13	1:B:475:LEU:H	1.72	0.55
1:B:180:THR:HG21	1:B:335:VAL:O	2.07	0.55
1:A:390:ILE:HD12	1:B:398:LYS:HE2	1.89	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: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
1:B:338:THR:O	1:B:338:THR:HG23	2.08	0.53
1:A:395:GLU:C	1:A:397:ILE:N	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:404:LYS:N	1:B:404:LYS:HE3	2.26	0.50
1:B:248:ILE:HG12	1:B:259:ILE:HD13	1.92	0.50
1:B:182:ILE:N	1:B:182:ILE:HD12	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:B:245:ARG:HB3	1:B:263:GLU:HG2	1.94	0.49
1:B:74:ILE:HA	1:B:78:HIS:O	2.13	0.49
1:A:231:GLU:O	1:A:235:THR:HB	2.13	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: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:264:LEU:HG	1:A:301:MET:CE	2.44	0.48
1:A:134:ILE:CG2	1:A:161:THR:HG23	2.39	0.48
1:A:366:THR:HG23	1:A:488:LEU:HD22	1.96	0.48
1:A:264:LEU:HG	1:A:301:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLU:O	1:A:396:MET:HB2	2.13	0.48
1:A:223:ILE:HG12	1:A:519:THR:HG21	1.95	0.48
1:B:380:LEU:HD23	1:B:383:LEU:HD12	1.96	0.48
1:A:101:MET:H	1:A:101:MET:HE3	1.78	0.48
1:B:274:ILE:HG22	1:B:292:LEU:HD13	1.96	0.48
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:509:ILE:HG13	1:A:510:ARG:N	2.29	0.47
1:B:413:GLN:HB2	1:B:415:TRP:CZ3	2.50	0.47
1:A:464:TYR:CB	1:B:459:VAL:HG13	2.42	0.47
1:B:396:MET:SD	1:B:409:LYS:O	2.72	0.47
1:B:461:LEU:HD11	1:B:465:LYS:HB2	1.97	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: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:395:GLU:HG2	1:A:396:MET:N	2.23	0.46
1:A:390:ILE:O	1:A:394:ILE:HG12	2.15	0.46
1:A:338:THR:HG23	1:A:339:ASN:N	2.30	0.46
1:B:180:THR:CG2	1:B:335:VAL:O	2.64	0.46
1:A:454:GLN:O	1:A:458:ILE:HD13	2.16	0.46
1:A:103:VAL:HG13	1:A:125:ILE:HG13	1.97	0.46
1:A:163:VAL:HG22	1:A:509:ILE:HD13	1.97	0.46
1:B:413:GLN:HB2	1:B:415:TRP:CH2	2.51	0.46
1:A:335:VAL:HA	1:A:343:LYS:O	2.15	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:99:ARG:HA	1:B:218:PRO:HB3	1.98	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:B:387:LEU:HA	1:B:390:ILE:CG1	2.44	0.46
1:B:80:HIS:C	1:B:82:ASP:H	2.18	0.46
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:264:LEU:HD12	1:B:301:MET:HE1	1.97	0.46
1:B:217:PHE:CE2	1:B:223:ILE:HD11	2.47	0.46
1:A:235:THR:HG22	1:A:237:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:GLU:O	1:B:410:LEU:HB2	2.16	0.45
1:B:59:TRP:HA	1:B:126:ARG:HG3	1.97	0.45
1:A:312:VAL:CG1	1:A:315:VAL:HG23	2.46	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:461:LEU:CD1	1:B:465:LYS:HB2	2.46	0.45
1:B:233:TYR:HB3	1:B:347:ILE:HG12	1.97	0.45
1:A:52:MET:HE3	1:A:125:ILE:HG23	1.99	0.45
1:A:451:THR:HB	2:A:556:HOH:O	2.17	0.45
1:A:104:ASP:OD2	1:A:126:ARG:HD3	2.16	0.45
1:B:386:ALA:CB	1:B:458:ILE:HD12	2.47	0.45
1:A:208:ILE:HD13	1:A:347:ILE:HG23	1.98	0.45
1:B:198:ILE:HD11	1:B:355:VAL:CG1	2.46	0.44
1:A:439:PRO:HB2	1:A:440:GLU:OE2	2.16	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: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:376:ARG:HG2	1:A:481:LEU:HD21	2.00	0.44
1:A:395:GLU:O	1:A:396:MET:CB	2.65	0.44
1:B:195:LEU:HA	1:B:195:LEU:HD23	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:A:396:MET:HE2	1:A:409:LYS:O	2.18	0.43
1:B:402:ASN:HD22	1:B:404:LYS:HB2	1.82	0.43
1:B:233:TYR:CB	1:B:347:ILE:HG12	2.48	0.43
1:B:264:LEU:HD21	1:B:303:MET:HE2	2.00	0.43
1:B:162:ARG:HG3	1:B:358:ARG:NH2	2.33	0.43
1:A:47:ARG:NH1	1:A:78:HIS:HD2	2.16	0.43
1:B:34:LEU:HD12	1:B:34:LEU:N	2.34	0.43
1:A:385:ILE:HD13	1:A:386:ALA:N	2.34	0.43
1:B:213:PRO:O	1:B:229:ILE:HG21	2.18	0.43
1:B:93:ALA:O	1:B:101:MET:HE3	2.19	0.43
1:B:233:TYR:HB3	1:B:347:ILE:CD1	2.49	0.43
1:B:219:THR:O	1:B:220:ALA:HB3	2.18	0.43
1:A:289:ILE:HD11	1:A:316:VAL:HG13	2.01	0.43
1:B:168:VAL:HG21	1:B:187:LEU:HD13	2.01	0.43
1:A:402:ASN:OD1	1:A:405:GLU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLU:CG	1:B:288:GLY:H	2.17	0.43
1:A:69:VAL:O	1:A:73:VAL:HG23	2.19	0.43
1:B:347:ILE:H	1:B:347:ILE:HG13	1.66	0.43
1:B:391:ASP:HB2	1:B:392:PRO:HD3	2.01	0.42
1:A:381:GLU:HG3	1:A:478:TYR:CZ	2.54	0.42
1:A:464:TYR:HA	1:B:397:ILE:HG21	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:273:LEU:HD21	1:A:326:MET:HE2	2.01	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: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:O	1:B:312:VAL:HG23	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:B:390:ILE:HG22	1:B:394:ILE:CD1	2.50	0.41
1:A:77:TYR:CD1	1:A:155:ILE:HD12	2.56	0.41
1:A:325:GLN:C	1:A:327:GLN:N	2.73	0.41
1:A:347:ILE:HG13	1:A:347:ILE:O	2.21	0.41
1:A:148:ASN:HB3	1:A:155:ILE:HD11	2.03	0.41
1:B:125:ILE:HG22	1:B:126:ARG:N	2.35	0.41
1:A:320:LEU:HD12	1:A:320:LEU:HA	1.85	0.41
1:A:395:GLU:HA	1:A:398:LYS:HG3	2.02	0.41
1:A:134:ILE:HG12	1:A:161:THR:HG23	2.03	0.41
1:A:180:THR:HG22	1:A:181:ASN:H	1.85	0.41
1:A:92:MET:HA	1:A:98:LEU:HD22	2.01	0.41
1:B:232:ALA:HB2	1:B:238:GLY:HA3	2.01	0.41
1:B:410:LEU:HD23	1:B:415:TRP:CH2	2.56	0.41
1:B:292:LEU:O	1:B:292:LEU:HD12	2.20	0.41
1:B:409:LYS:HD3	1:B:412:SER:OG	2.21	0.41
1:A:53:ASP:HB2	1:A:135:LEU:HD12	2.02	0.41
1:A:389:ASN:HD21	1:A:415:TRP:HD1	1.69	0.40
1:B:406:SER:O	1:B:410:LEU:HG	2.21	0.40
1:B:86:TYR:OH	1:B:123:THR:HG21	2.22	0.40
1:B:484:LEU:O	1:B:484:LEU:HD22	2.22	0.40
1:A:438:GLU:O	1:A:440:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ILE:HG21	1:B:510:ARG:HB2	2.03	0.40
1:A:237:ARG:HA	1:A:332:LEU:O	2.22	0.40
1:A:180:THR:CG2	1:A:335:VAL:H	2.24	0.40
1:B:259:ILE:HB	1:B:305:ILE:HG23	2.03	0.40
1:A:232:ALA:HB2	1:A:238:GLY:HA3	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 [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	454/500 (91%)	430 (95%)	21 (5%)	3 (1%)	26	51
1	B	448/500 (90%)	410 (92%)	30 (7%)	8 (2%)	11	21
All	All	902/1000 (90%)	840 (93%)	51 (6%)	11 (1%)	16	33

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 ⓘ

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%)	357 (91%)	37 (9%)	11	20
1	B	390/424 (92%)	358 (92%)	32 (8%)	14	27
All	All	784/848 (92%)	715 (91%)	69 (9%)	12	24

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	60	ASN
1	A	101	MET
1	A	121	ARG
1	A	126	ARG
1	A	135	LEU
1	A	154	HIS
1	A	155	ILE
1	A	161	THR
1	A	168	VAL
1	A	180	THR
1	A	219	THR
1	A	231	GLU
1	A	241	LYS
1	A	256	LYS
1	A	259	ILE
1	A	270	LYS
1	A	275	GLU
1	A	276	LYS
1	A	285	ARG
1	A	298	LYS
1	A	309	ARG
1	A	318	ASN
1	A	320	LEU
1	A	347	ILE
1	A	372	LYS
1	A	385	ILE

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Mol	Chain	Res	Type
1	A	390	ILE
1	A	415	TRP
1	A	439	PRO
1	A	461	LEU
1	A	463	LEU
1	A	473	LYS
1	A	484	LEU
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	180	THR
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	283	ASP
1	B	286	LEU
1	B	298	LYS
1	B	305	ILE
1	B	332	LEU
1	B	347	ILE
1	B	389	ASN
1	B	390	ILE
1	B	401	ASN
1	B	404	LYS
1	B	409	LYS
1	B	474	ILE
1	B	484	LEU
1	B	485	ILE
1	B	487	GLU
1	B	512	GLU
1	B	516	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	267	GLN
1	A	318	ASN
1	A	339	ASN
1	A	413	GLN
1	A	471	HIS
1	B	57	ASN
1	B	106	GLN
1	B	169	ASN
1	B	181	ASN
1	B	185	HIS
1	B	262	HIS
1	B	319	ASN
1	B	333	ASN
1	B	357	HIS
1	B	389	ASN
1	B	401	ASN
1	B	402	ASN
1	B	413	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.23	12 (2%) 59 53	32, 47, 70, 87	0
1	B	458/500 (91%)	0.32	23 (5%) 32 26	31, 47, 74, 87	0
All	All	920/1000 (92%)	0.27	35 (3%) 44 36	31, 47, 72, 87	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	ILE	8.2
1	B	397	ILE	5.8
1	B	401	ASN	4.8
1	B	393	ILE	4.5
1	A	412	SER	4.1
1	A	411	ILE	4.0
1	A	397	ILE	3.5
1	B	463	LEU	3.5
1	B	412	SER	3.3
1	B	385	ILE	3.1
1	B	81	GLY	3.0
1	B	466	LEU	3.0
1	B	407	GLU	2.9
1	A	388	ALA	2.8
1	B	408	GLU	2.7
1	B	309	ARG	2.7
1	A	299	ASP	2.7
1	B	475	LEU	2.7
1	B	416	GLU	2.7
1	A	406	SER	2.6
1	B	405	GLU	2.6
1	A	401	ASN	2.5
1	B	479	LYS	2.5
1	B	455	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	468	GLY	2.5
1	A	458	ILE	2.5
1	A	405	GLU	2.5
1	B	460	ASP	2.4
1	B	469	MET	2.3
1	B	464	TYR	2.3
1	A	478	TYR	2.2
1	B	410	LEU	2.2
1	B	389	ASN	2.2
1	A	341	GLN	2.1
1	A	482	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.