Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2025 – 10:05 AM EDT

PDB ID	:	9NT3 / pdb_00009nt3
Title	:	Crystal structure of apo ecLacI transcription factor ancestor 1
Authors	:	Georgelin, R.L.; Frkic, R.L.; Jackson, C.J.
Deposited on	:	2025-03-18
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:

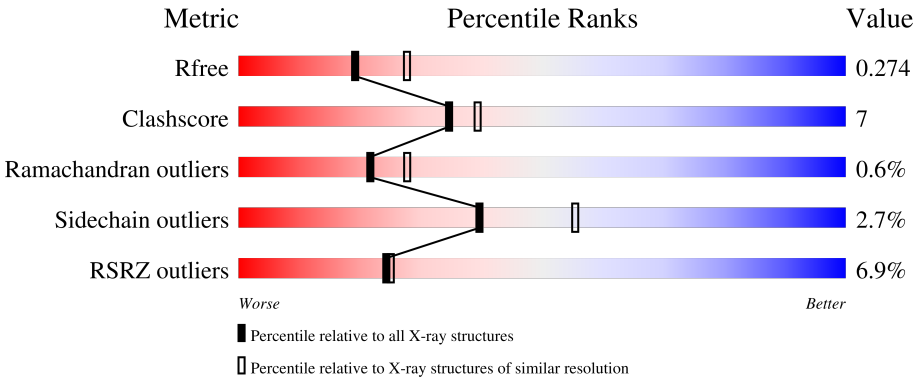
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (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 <=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	280	10% 70% 21% 8%
1	B	280	10% 73% 20% 7%
1	C	280	5% 79% 15% 6%
1	D	280	% 82% 10% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8184 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 Ancestral LacI Transcription Factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	263	Total	C	N	O	S	0	0	0
			2033	1281	354	396	2			
1	A	259	Total	C	N	O	S	0	0	0
			2019	1279	354	384	2			
1	C	263	Total	C	N	O	S	0	0	0
			2039	1293	353	391	2			
1	B	260	Total	C	N	O	S	0	0	0
			2014	1281	348	383	2			

- Molecule 2 is water.

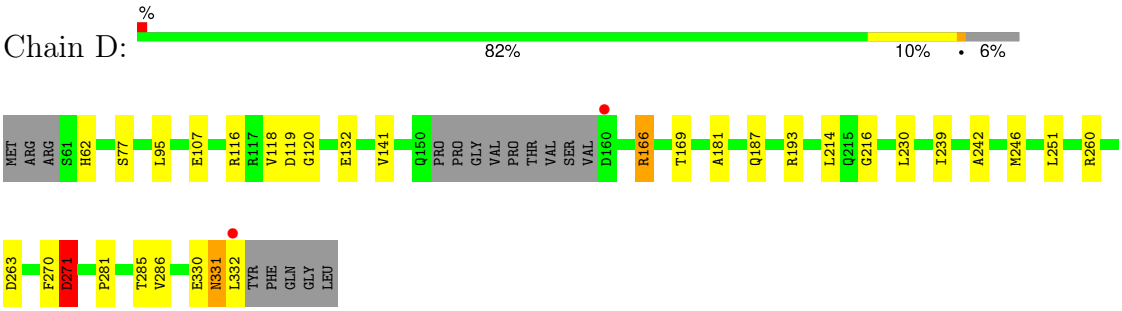
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	27	Total	O	0	0
			27	27		
2	A	16	Total	O	0	0
			16	16		
2	C	21	Total	O	0	0
			21	21		
2	B	15	Total	O	0	0
			15	15		

3 Residue-property plots (i)

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.

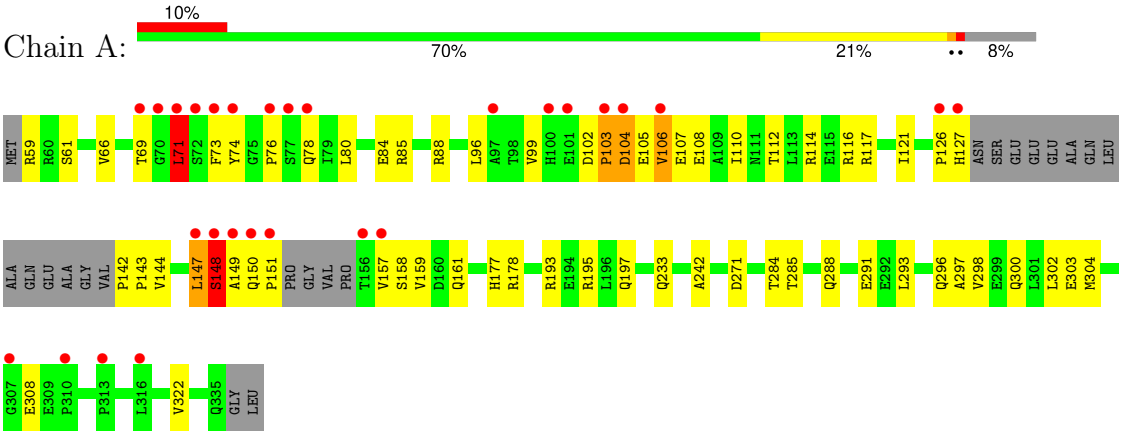
• Molecule 1: Ancestral LacI Transcription Factor

Chain D:



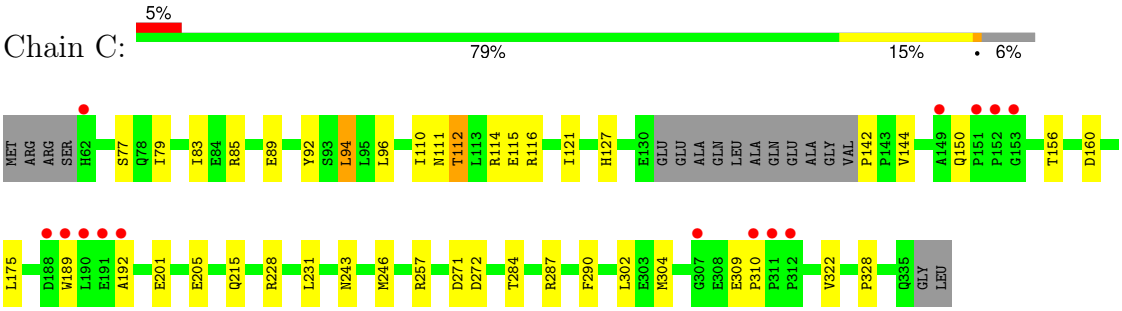
• Molecule 1: Ancestral LacI Transcription Factor

Chain A:



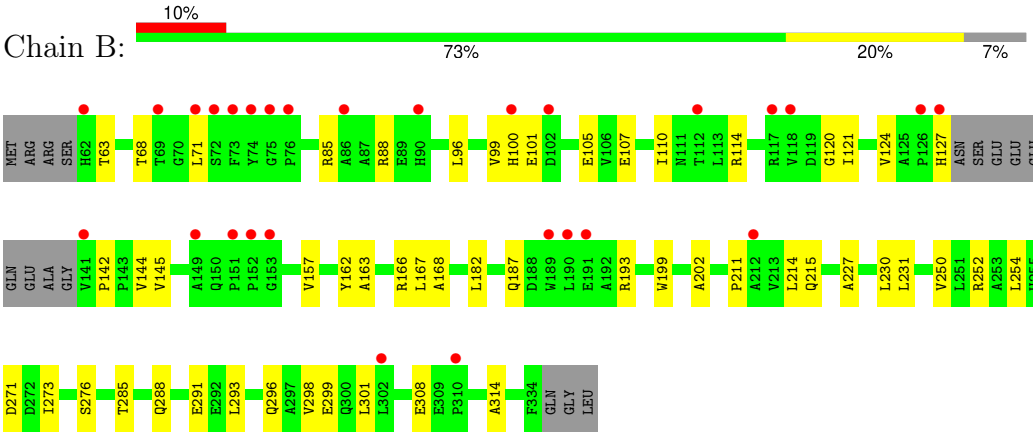
• Molecule 1: Ancestral LacI Transcription Factor

Chain C:



• Molecule 1: Ancestral LacI Transcription Factor

Chain B:


10%
73%
20%
7%
MET ARG ARG SER H62 T63 T68 T69 G70 L71 S72 F73 Y74 G75 P76 R85 A86 A87 R88 E89 H90 L96 V99 H100 E101 D102 E105 V106 E107 I110 N111 T112 L113 R114 R117 V118 D119 G120 I121 V124 A125 P126 H127 ASN SER GLU GLU GLU ALA GLN LEU ALA
GLN GLU ALA GLY V141 P142 P143 V144 V145 A149 Q150 P151 P152 G153 V157 Y162 A163 R166 L167 A168 L182 Q187 D188 W189 L190 E191 A192 R193 W199 A202 P211 A212 V213 L214 Q215 A227 L230 L231 V250 L251 R252 A253 L254 H255 E256 V268
D271 D272 I273 S276 T285 Q288 E291 E292 L293 Q296 A297 V298 E299 Q300 L301 L302 E308 E309 P310 A314 F334 GLN GLY LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.86Å 85.59Å 211.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.79 – 2.45 42.79 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.79-2.45) 99.9 (42.79-2.45)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.224 , 0.274 0.224 , 0.274	Depositor DCC
R_{free} test set	2112 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 28.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8184	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.23	0/2067	0.45	1/2823 (0.0%)
1	B	0.20	0/2065	0.39	0/2828
1	C	0.21	0/2090	0.38	0/2860
1	D	0.22	0/2079	0.39	0/2841
All	All	0.22	0/8301	0.40	1/11352 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	LEU	CA-CB-CG	5.60	135.91	116.30

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	2019	0	1978	46	0
1	B	2014	0	1974	33	0
1	C	2039	0	1991	25	0
1	D	2033	0	1978	20	0
2	A	16	0	0	1	0
2	B	15	0	0	0	0
2	C	21	0	0	0	0
2	D	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8184	0	7921	119	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 7.

All (119) 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:A:96:LEU:HB2	1:B:96:LEU:HB2	1.62	0.82
1:C:114:ARG:HD3	1:C:142:PRO:HD2	1.67	0.76
1:B:157:VAL:HG23	1:B:314:ALA:HB3	1.69	0.74
1:B:107:GLU:OE1	1:B:127:HIS:NE2	2.26	0.68
1:A:103:PRO:O	1:A:105:GLU:N	2.30	0.65
1:B:157:VAL:HG13	1:B:293:LEU:HD12	1.80	0.63
1:D:181:ALA:HB3	1:D:239:ILE:HG12	1.85	0.58
1:B:145:VAL:HG12	1:B:301:LEU:HD13	1.85	0.58
1:A:107:GLU:HG2	1:A:127:HIS:NE2	2.19	0.57
1:C:92:TYR:CE2	1:C:302:LEU:HD21	2.40	0.57
1:B:199:TRP:CZ2	1:B:211:PRO:HD2	2.40	0.57
1:C:121:ILE:HB	1:C:144:VAL:HG22	1.88	0.56
1:C:189:TRP:HB3	1:C:192:ALA:HB2	1.87	0.56
1:B:120:GLY:HA3	1:B:301:LEU:HD21	1.88	0.55
1:A:99:VAL:HG13	1:A:105:GLU:CD	2.32	0.55
1:C:110:ILE:HG23	1:C:121:ILE:HD12	1.90	0.54
1:B:110:ILE:HG22	1:B:121:ILE:HG21	1.88	0.54
1:A:66:VAL:HB	1:A:96:LEU:HD22	1.90	0.54
1:B:182:LEU:HD13	1:B:199:TRP:CG	2.43	0.54
1:C:89:GLU:OE2	1:B:88:ARG:NH2	2.41	0.54
1:D:271:ASP:O	1:D:285:THR:HG21	2.08	0.54
1:A:304:MET:HA	1:A:308:GLU:HA	1.90	0.53
1:A:103:PRO:C	1:A:105:GLU:H	2.16	0.53
1:D:107:GLU:HB2	1:D:132:GLU:HG3	1.89	0.53
1:C:150:GLN:H	1:C:156:THR:HG21	1.74	0.53
1:A:143:PRO:HB3	1:A:304:MET:HE2	1.90	0.53
1:B:271:ASP:OD1	1:B:288:GLN:NE2	2.41	0.53
1:C:304:MET:HE3	1:C:310:PRO:HG3	1.90	0.52
1:B:114:ARG:HG2	1:B:142:PRO:HG2	1.91	0.52
1:A:84:GLU:CD	1:A:88:ARG:HH12	2.18	0.52
1:B:166:ARG:HG3	1:B:202:ALA:HB2	1.92	0.52
1:B:187:GLN:O	1:B:193:ARG:NH2	2.42	0.52
1:A:104:ASP:O	1:A:108:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.76	0.51
1:D:166:ARG:NH2	2:D:404:HOH:O	2.44	0.51
1:A:116:ARG:NH2	1:B:63:THR:HG21	2.26	0.51
1:A:73:PHE:HD2	1:A:76:PRO:HG2	1.75	0.51
1:A:126:PRO:HB3	1:A:149:ALA:HB3	1.94	0.50
1:A:99:VAL:HG11	1:A:106:VAL:HG22	1.93	0.50
1:C:272:ASP:OD2	1:C:287:ARG:NH1	2.45	0.50
1:A:195:ARG:NH1	1:A:242:ALA:O	2.45	0.50
1:A:84:GLU:OE2	1:A:88:ARG:NH1	2.37	0.49
1:B:68:THR:HA	1:B:124:VAL:HG22	1.95	0.49
1:D:214:LEU:HD12	1:D:230:LEU:HG	1.94	0.49
1:A:114:ARG:CZ	1:A:142:PRO:HD2	2.42	0.49
1:D:62:HIS:N	1:D:119:ASP:OD2	2.42	0.49
1:D:118:VAL:HG12	1:D:120:GLY:H	1.77	0.49
1:D:251:LEU:HD22	1:D:281:PRO:HD2	1.93	0.49
1:D:285:THR:HG22	1:D:286:VAL:N	2.28	0.49
1:C:111:ASN:O	1:C:115:GLU:HG3	2.13	0.48
1:C:243:ASN:OD1	1:C:246:MET:HG3	2.13	0.48
1:B:214:LEU:HD12	1:B:230:LEU:HG	1.94	0.48
1:A:177:HIS:O	1:A:178:ARG:NH1	2.46	0.48
1:A:284:THR:HG23	1:A:322:VAL:HA	1.95	0.48
1:C:114:ARG:HH11	1:C:142:PRO:HD2	1.78	0.48
1:C:284:THR:HG23	1:C:322:VAL:HA	1.94	0.48
1:A:71:LEU:C	1:A:73:PHE:H	2.22	0.48
1:C:309:GLU:OE1	1:C:309:GLU:N	2.42	0.48
1:C:127:HIS:O	1:C:150:GLN:NE2	2.38	0.47
1:A:110:ILE:HG23	1:A:121:ILE:HD12	1.96	0.47
1:A:110:ILE:O	1:A:114:ARG:HG3	2.15	0.47
1:A:303:GLU:O	1:A:308:GLU:N	2.39	0.47
1:D:166:ARG:NH1	1:D:169:THR:OG1	2.47	0.47
1:A:159:VAL:HG11	1:A:288:GLN:HB3	1.95	0.47
1:B:110:ILE:O	1:B:114:ARG:N	2.45	0.47
1:A:296:GLN:O	1:A:300:GLN:HG2	2.15	0.46
1:D:95:LEU:HD21	1:D:116:ARG:HG3	1.97	0.46
1:A:74:TYR:CZ	1:A:78:GLN:HG3	2.50	0.46
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.78	0.45
1:B:121:ILE:HB	1:B:144:VAL:HG12	1.98	0.45
1:B:182:LEU:HB2	1:B:199:TRP:CE2	2.52	0.45
1:D:181:ALA:HB1	1:D:230:LEU:HD13	1.98	0.45
1:A:233:GLN:HB3	2:A:406:HOH:O	2.17	0.45
1:B:163:ALA:O	1:B:167:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ARG:HA	1:D:166:ARG:HH11	1.81	0.45
1:D:166:ARG:HA	1:D:166:ARG:HD3	1.73	0.45
1:A:59:ARG:HB3	1:A:59:ARG:NH1	2.31	0.45
1:A:147:LEU:HD21	1:A:297:ALA:HB2	1.99	0.45
1:A:117:ARG:HG3	1:A:117:ARG:NH1	2.33	0.44
1:C:201:GLU:O	1:C:205:GLU:HG2	2.17	0.44
1:B:252:ARG:O	1:B:256:GLU:HG3	2.18	0.44
1:A:61:SER:HB3	1:A:117:ARG:HD3	2.00	0.44
1:C:96:LEU:HD23	1:C:96:LEU:HA	1.81	0.44
1:A:103:PRO:O	1:A:105:GLU:HG2	2.17	0.44
1:C:85:ARG:HH22	1:B:85:ARG:HH12	1.67	0.43
1:A:271:ASP:O	1:A:285:THR:OG1	2.26	0.43
1:A:80:LEU:HD23	1:B:71:LEU:HD11	2.00	0.43
1:A:159:VAL:HG23	1:A:293:LEU:HD22	2.01	0.43
1:C:79:ILE:HG13	1:C:290:PHE:CD1	2.54	0.43
1:A:85:ARG:NH1	1:A:291:GLU:OE2	2.51	0.43
1:B:273:ILE:HG12	1:B:276:SER:HB3	2.00	0.43
1:C:175:LEU:HD22	1:C:328:PRO:HD3	2.00	0.43
1:B:168:ALA:HB1	1:B:268:VAL:HG11	2.00	0.43
1:A:298:VAL:O	1:A:302:LEU:HG	2.19	0.43
1:B:231:LEU:HD11	1:B:254:LEU:HD23	1.99	0.43
1:C:287:ARG:HH11	1:C:287:ARG:HG3	1.84	0.43
1:D:187:GLN:HE22	1:D:193:ARG:HA	1.84	0.42
1:C:83:ILE:HG22	1:C:94:LEU:HD11	2.02	0.42
1:A:193:ARG:O	1:A:197:GLN:HG2	2.19	0.42
1:D:216:GLY:HA3	1:D:246:MET:SD	2.60	0.42
1:A:148:SER:HB3	1:A:149:ALA:H	1.59	0.42
1:B:99:VAL:HG13	1:B:105:GLU:HB3	2.01	0.42
1:B:100:HIS:HB3	1:B:101:GLU:H	1.67	0.42
1:A:73:PHE:HB2	1:A:76:PRO:HD2	2.00	0.42
1:B:162:TYR:OH	1:B:166:ARG:NH1	2.52	0.42
1:B:227:ALA:HB2	1:B:250:VAL:HG22	2.02	0.42
1:C:231:LEU:HD13	1:C:257:ARG:HD2	2.02	0.41
1:D:187:GLN:NE2	1:D:193:ARG:HG2	2.35	0.41
1:D:331:ASN:O	1:D:332:LEU:HG	2.20	0.41
1:D:260:ARG:HB2	1:D:263:ASP:HB2	2.03	0.41
1:C:112:THR:O	1:C:116:ARG:HD2	2.20	0.41
1:B:271:ASP:O	1:B:285:THR:OG1	2.24	0.41
1:A:69:THR:HA	1:A:99:VAL:O	2.21	0.40
1:A:59:ARG:HB3	1:A:59:ARG:HH11	1.85	0.40
1:A:161:GLN:NE2	1:A:288:GLN:HE22	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ALA:O	1:D:270:PHE:HB3	2.22	0.40
1:A:121:ILE:HB	1:A:144:VAL:HG22	2.04	0.40
1:A:150:GLN:HB2	1:A:151:PRO:HD2	2.02	0.40
1:B:296:GLN:HA	1:B:299:GLU:HB2	2.03	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	253/280 (90%)	238 (94%)	12 (5%)	3 (1%)	11 11
1	B	256/280 (91%)	237 (93%)	19 (7%)	0	100 100
1	C	259/280 (92%)	247 (95%)	11 (4%)	1 (0%)	30 38
1	D	259/280 (92%)	252 (97%)	5 (2%)	2 (1%)	16 21
All	All	1027/1120 (92%)	974 (95%)	47 (5%)	6 (1%)	22 28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASP
1	A	148	SER
1	D	271	ASP
1	D	331	ASN
1	A	103	PRO
1	C	160	ASP

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	213/228 (93%)	205 (96%)	8 (4%)	28	41
1	B	213/228 (93%)	209 (98%)	4 (2%)	52	67
1	C	216/228 (95%)	210 (97%)	6 (3%)	38	54
1	D	213/228 (93%)	208 (98%)	5 (2%)	45	61
All	All	855/912 (94%)	832 (97%)	23 (3%)	40	55

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	77	SER
1	D	141	VAL
1	D	166	ARG
1	D	271	ASP
1	D	330	GLU
1	A	71	LEU
1	A	102	ASP
1	A	106	VAL
1	A	112	THR
1	A	147	LEU
1	A	148	SER
1	A	157	VAL
1	A	158	SER
1	C	77	SER
1	C	94	LEU
1	C	112	THR
1	C	215	GLN
1	C	228	ARG
1	C	271	ASP
1	B	215	GLN
1	B	291	GLU
1	B	298	VAL
1	B	308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	134	GLN
1	D	187	GLN
1	D	288	GLN
1	A	187	GLN
1	A	215	GLN
1	A	288	GLN
1	A	331	ASN
1	C	197	GLN
1	C	215	GLN
1	B	197	GLN
1	B	255	HIS

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 oligosaccharides 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, 95^{th} 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	259/280 (92%)	0.25	28 (10%)	12	12	23, 45, 103, 136	0
1	B	260/280 (92%)	0.55	28 (10%)	12	12	26, 60, 105, 143	0
1	C	263/280 (93%)	0.31	14 (5%)	33	33	25, 49, 91, 111	0
1	D	263/280 (93%)	-0.21	2 (0%)	82	83	24, 40, 61, 79	0
All	All	1045/1120 (93%)	0.22	72 (6%)	24	25	23, 46, 97, 143	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	PHE	5.6
1	C	189	TRP	4.8
1	C	190	LEU	4.7
1	A	72	SER	4.5
1	A	147	LEU	4.3
1	C	153	GLY	3.8
1	A	156	THR	3.7
1	A	151	PRO	3.7
1	A	74	TYR	3.4
1	C	191	GLU	3.2
1	B	126	PRO	3.2
1	A	148	SER	3.2
1	B	141	VAL	3.2
1	A	77	SER	3.1
1	A	103	PRO	3.1
1	C	312	PRO	3.1
1	A	149	ALA	3.1
1	B	74	TYR	3.1
1	C	311	PRO	3.0
1	B	69	THR	3.0
1	B	71	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	3.0
1	A	71	LEU	2.9
1	A	76	PRO	2.9
1	D	332	LEU	2.9
1	A	126	PRO	2.9
1	B	149	ALA	2.9
1	B	152	PRO	2.8
1	A	101	GLU	2.8
1	B	112	THR	2.7
1	A	127	HIS	2.7
1	C	149	ALA	2.7
1	B	90	HIS	2.7
1	A	150	GLN	2.6
1	B	62	HIS	2.6
1	B	153	GLY	2.6
1	B	72	SER	2.6
1	B	75	GLY	2.5
1	A	316	LEU	2.5
1	B	127	HIS	2.5
1	C	192	ALA	2.5
1	D	160	ASP	2.5
1	A	104	ASP	2.5
1	A	310	PRO	2.5
1	C	151	PRO	2.5
1	C	152	PRO	2.5
1	A	100	HIS	2.4
1	C	188	ASP	2.4
1	B	73	PHE	2.4
1	B	151	PRO	2.4
1	B	100	HIS	2.4
1	B	118	VAL	2.3
1	A	97	ALA	2.3
1	A	313	PRO	2.3
1	B	212	ALA	2.3
1	B	189	TRP	2.2
1	B	310	PRO	2.2
1	A	78	GLN	2.2
1	C	310	PRO	2.2
1	A	70	GLY	2.2
1	B	76	PRO	2.2
1	C	307	GLY	2.2
1	B	86	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	191	GLU	2.1
1	B	102	ASP	2.1
1	A	157	VAL	2.1
1	B	190	LEU	2.1
1	B	302	LEU	2.1
1	C	62	HIS	2.0
1	A	106	VAL	2.0
1	B	117	ARG	2.0
1	A	307	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 monosaccharides 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.