



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:40 AM EDT

PDB ID : 1L3A
Title : Structure of the plant transcriptional regulator PBF-2
Authors : Desveaux, D.; Allard, J.; Brisson, N.; Sygusch, J.
Deposited on : 2002-02-26
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

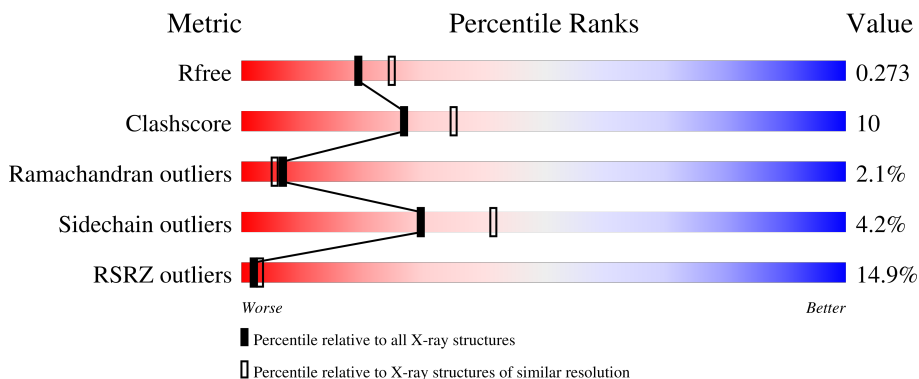
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	227	
1	B	227	
1	C	227	
1	D	227	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5912 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 p24: plant transcriptional regulator PBF-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	166	1307	847	218	238	4	0	0	0
1	B	170	1338	866	222	246	4	0	0	0
1	C	182	1448	933	248	263	4	0	0	0
1	D	171	1342	868	223	247	4	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	cloning artifact	UNP Q9LL85
A	56	ALA	-	cloning artifact	UNP Q9LL85
A	57	SER	-	cloning artifact	UNP Q9LL85
A	58	MET	-	cloning artifact	UNP Q9LL85
A	59	THR	-	cloning artifact	UNP Q9LL85
A	60	GLY	-	cloning artifact	UNP Q9LL85
A	61	GLY	-	cloning artifact	UNP Q9LL85
A	62	GLN	-	cloning artifact	UNP Q9LL85
A	63	GLN	-	cloning artifact	UNP Q9LL85
A	64	MET	-	cloning artifact	UNP Q9LL85
A	65	GLY	-	cloning artifact	UNP Q9LL85
A	66	ARG	-	cloning artifact	UNP Q9LL85
A	67	GLY	-	cloning artifact	UNP Q9LL85
A	166	THR	-	engineered mutation	UNP Q9LL85
A	274	LEU	-	cloning artifact	UNP Q9LL85
A	275	GLU	-	cloning artifact	UNP Q9LL85
A	276	HIS	-	expression tag	UNP Q9LL85
A	277	HIS	-	expression tag	UNP Q9LL85
A	278	HIS	-	expression tag	UNP Q9LL85
A	279	HIS	-	expression tag	UNP Q9LL85
A	280	HIS	-	expression tag	UNP Q9LL85

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Chain	Residue	Modelled	Actual	Comment	Reference
A	281	HIS	-	expression tag	UNP Q9LL85
B	55	MET	-	cloning artifact	UNP Q9LL85
B	56	ALA	-	cloning artifact	UNP Q9LL85
B	57	SER	-	cloning artifact	UNP Q9LL85
B	58	MET	-	cloning artifact	UNP Q9LL85
B	59	THR	-	cloning artifact	UNP Q9LL85
B	60	GLY	-	cloning artifact	UNP Q9LL85
B	61	GLY	-	cloning artifact	UNP Q9LL85
B	62	GLN	-	cloning artifact	UNP Q9LL85
B	63	GLN	-	cloning artifact	UNP Q9LL85
B	64	MET	-	cloning artifact	UNP Q9LL85
B	65	GLY	-	cloning artifact	UNP Q9LL85
B	66	ARG	-	cloning artifact	UNP Q9LL85
B	67	GLY	-	cloning artifact	UNP Q9LL85
B	166	THR	-	engineered mutation	UNP Q9LL85
B	274	LEU	-	cloning artifact	UNP Q9LL85
B	275	GLU	-	cloning artifact	UNP Q9LL85
B	276	HIS	-	expression tag	UNP Q9LL85
B	277	HIS	-	expression tag	UNP Q9LL85
B	278	HIS	-	expression tag	UNP Q9LL85
B	279	HIS	-	expression tag	UNP Q9LL85
B	280	HIS	-	expression tag	UNP Q9LL85
B	281	HIS	-	expression tag	UNP Q9LL85
C	55	MET	-	cloning artifact	UNP Q9LL85
C	56	ALA	-	cloning artifact	UNP Q9LL85
C	57	SER	-	cloning artifact	UNP Q9LL85
C	58	MET	-	cloning artifact	UNP Q9LL85
C	59	THR	-	cloning artifact	UNP Q9LL85
C	60	GLY	-	cloning artifact	UNP Q9LL85
C	61	GLY	-	cloning artifact	UNP Q9LL85
C	62	GLN	-	cloning artifact	UNP Q9LL85
C	63	GLN	-	cloning artifact	UNP Q9LL85
C	64	MET	-	cloning artifact	UNP Q9LL85
C	65	GLY	-	cloning artifact	UNP Q9LL85
C	66	ARG	-	cloning artifact	UNP Q9LL85
C	67	GLY	-	cloning artifact	UNP Q9LL85
C	166	THR	-	engineered mutation	UNP Q9LL85
C	274	LEU	-	cloning artifact	UNP Q9LL85
C	275	GLU	-	cloning artifact	UNP Q9LL85
C	276	HIS	-	expression tag	UNP Q9LL85
C	277	HIS	-	expression tag	UNP Q9LL85
C	278	HIS	-	expression tag	UNP Q9LL85

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Chain	Residue	Modelled	Actual	Comment	Reference
C	279	HIS	-	expression tag	UNP Q9LL85
C	280	HIS	-	expression tag	UNP Q9LL85
C	281	HIS	-	expression tag	UNP Q9LL85
D	55	MET	-	cloning artifact	UNP Q9LL85
D	56	ALA	-	cloning artifact	UNP Q9LL85
D	57	SER	-	cloning artifact	UNP Q9LL85
D	58	MET	-	cloning artifact	UNP Q9LL85
D	59	THR	-	cloning artifact	UNP Q9LL85
D	60	GLY	-	cloning artifact	UNP Q9LL85
D	61	GLY	-	cloning artifact	UNP Q9LL85
D	62	GLN	-	cloning artifact	UNP Q9LL85
D	63	GLN	-	cloning artifact	UNP Q9LL85
D	64	MET	-	cloning artifact	UNP Q9LL85
D	65	GLY	-	cloning artifact	UNP Q9LL85
D	66	ARG	-	cloning artifact	UNP Q9LL85
D	67	GLY	-	cloning artifact	UNP Q9LL85
D	166	THR	-	engineered mutation	UNP Q9LL85
D	274	LEU	-	cloning artifact	UNP Q9LL85
D	275	GLU	-	cloning artifact	UNP Q9LL85
D	276	HIS	-	expression tag	UNP Q9LL85
D	277	HIS	-	expression tag	UNP Q9LL85
D	278	HIS	-	expression tag	UNP Q9LL85
D	279	HIS	-	expression tag	UNP Q9LL85
D	280	HIS	-	expression tag	UNP Q9LL85
D	281	HIS	-	expression tag	UNP Q9LL85

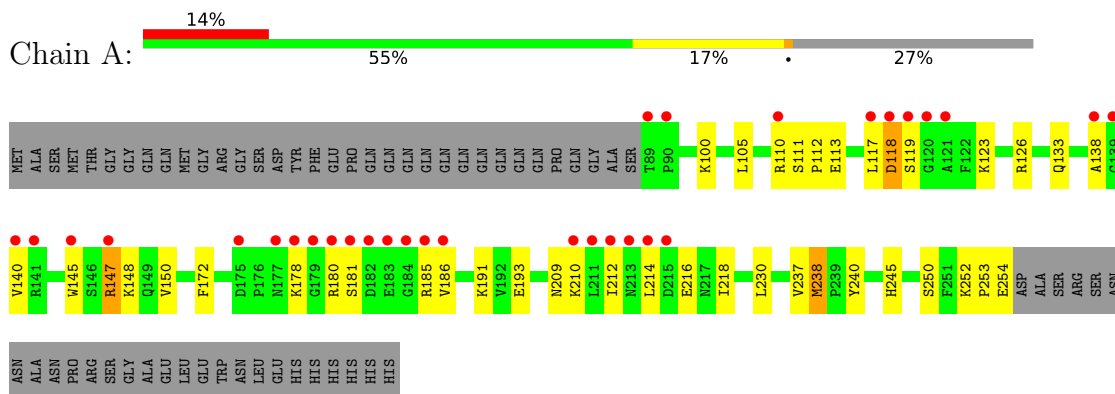
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	105	Total O 105 105	0	0
2	B	94	Total O 94 94	0	0
2	C	150	Total O 150 150	0	0
2	D	128	Total O 128 128	0	0

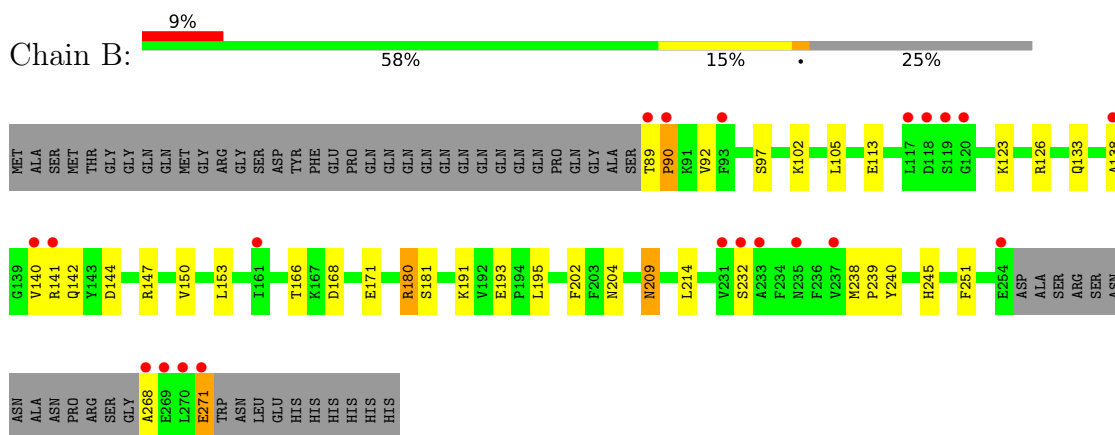
3 Residue-property plots

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.

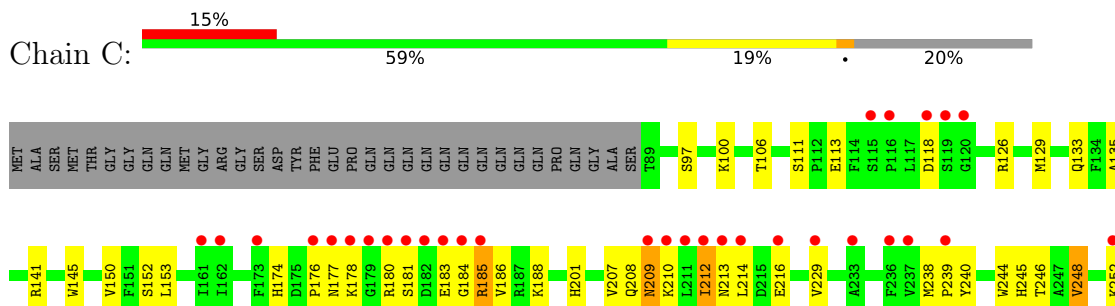
- Molecule 1: p24: plant transcriptional regulator PBF-2

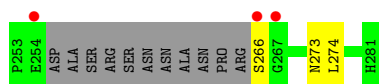


- Molecule 1: p24: plant transcriptional regulator PBF-2

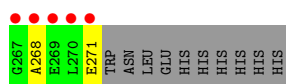
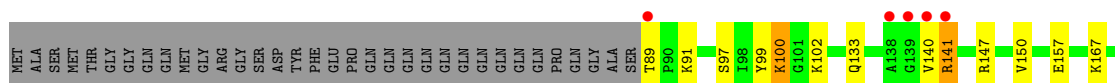


- Molecule 1: p24: plant transcriptional regulator PBF-2





- Molecule 1: p24: plant transcriptional regulator PBF-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.87Å 89.81Å 144.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.42 – 2.30 42.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.9 (42.42-2.30) 89.8 (42.42-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.72 (at 2.29Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.267 0.222 , 0.273	Depositor DCC
R_{free} test set	4062 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtrriage
Anisotropy	0.373	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5912	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/1342	0.56	0/1817
1	B	0.42	0/1372	0.57	0/1856
1	C	0.42	0/1490	0.57	0/2016
1	D	0.44	0/1376	0.60	0/1861
All	All	0.42	0/5580	0.58	0/7550

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1307	0	1303	28	0
1	B	1338	0	1330	33	0
1	C	1448	0	1413	36	0
1	D	1342	0	1333	24	0
2	A	105	0	0	5	0
2	B	94	0	0	4	0
2	C	150	0	0	3	0
2	D	128	0	0	5	0
All	All	5912	0	5379	110	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 10.

All (110) 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:238:MET:HE1	1:D:229:VAL:HG22	1.48	0.94
1:A:185:ARG:HD3	1:A:210:LYS:HB3	1.53	0.87
1:A:133:GLN:HG2	1:A:150:VAL:HG12	1.60	0.83
1:B:180:ARG:HH11	1:B:180:ARG:HB3	1.42	0.81
1:C:180:ARG:HG2	1:C:181:SER:H	1.46	0.80
1:B:140:VAL:HG13	1:B:141:ARG:H	1.47	0.79
1:D:133:GLN:HG2	1:D:150:VAL:HG12	1.66	0.77
1:A:253:PRO:O	1:A:254:GLU:HB2	1.82	0.77
1:D:193:GLU:HB2	2:D:403:HOH:O	1.91	0.71
1:D:89:THR:N	1:D:91:LYS:HZ2	1.88	0.70
1:C:209:ASN:HD21	1:C:212:ILE:HG13	1.58	0.67
1:A:186:VAL:HG22	1:A:209:ASN:HB2	1.76	0.67
1:D:177:ASN:O	1:D:183:GLU:HB3	1.96	0.65
1:C:209:ASN:OD1	1:C:212:ILE:HB	1.97	0.65
1:B:126:ARG:HH21	1:C:266:SER:N	1.94	0.64
1:C:188:LYS:NZ	1:D:271:GLU:HB2	2.12	0.63
1:C:183:GLU:HG3	1:C:184:GLY:N	2.13	0.63
1:D:202:PHE:HB2	2:D:403:HOH:O	1.99	0.63
1:A:110:ARG:HD2	2:A:360:HOH:O	1.98	0.62
1:B:166:THR:O	2:B:305:HOH:O	2.16	0.61
1:B:123:LYS:HB3	1:B:123:LYS:NZ	2.15	0.61
1:C:113:GLU:HB2	1:C:126:ARG:HB3	1.82	0.61
1:B:193:GLU:HB2	1:B:202:PHE:CZ	2.38	0.58
1:A:113:GLU:HB3	1:A:126:ARG:HB3	1.87	0.56
1:C:133:GLN:HG2	1:C:150:VAL:HG22	1.86	0.56
1:B:209:ASN:C	1:B:209:ASN:HD22	2.09	0.56
1:C:97:SER:OG	1:C:106:THR:HG22	2.05	0.55
1:C:183:GLU:HG3	1:C:184:GLY:H	1.71	0.55
1:C:214:LEU:HD11	1:C:216:GLU:HG3	1.89	0.55
1:D:99:TYR:O	1:D:100:LYS:HD2	2.08	0.54
1:C:188:LYS:HZ2	1:D:271:GLU:HB2	1.71	0.54
1:C:111:SER:HB2	1:D:251:PHE:CD2	2.42	0.54
1:D:157:GLU:OE2	1:D:174:HIS:HE1	1.91	0.54
1:A:191:LYS:HE3	1:A:193:GLU:CD	2.28	0.54
1:C:152:SER:O	1:C:174:HIS:HE1	1.90	0.53
1:D:240:TYR:HA	1:D:245:HIS:CD2	2.44	0.53
1:C:177:ASN:ND2	1:C:180:ARG:HD2	2.24	0.52
1:A:118:ASP:HB2	2:A:366:HOH:O	2.09	0.52
1:B:144:ASP:OD2	1:B:147:ARG:HG2	2.10	0.51
1:B:171:GLU:OE2	1:B:191:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ALA:HB2	1:B:144:ASP:HB2	1.92	0.51
1:C:201:HIS:HD2	2:C:304:HOH:O	1.93	0.51
1:C:180:ARG:HG2	1:C:181:SER:N	2.21	0.50
1:C:113:GLU:OE1	1:C:126:ARG:HD2	2.12	0.49
1:A:172:PHE:HD2	2:A:313:HOH:O	1.95	0.49
1:B:209:ASN:HB3	1:B:214:LEU:HB3	1.94	0.49
1:B:142:GLN:HG2	2:B:364:HOH:O	2.12	0.49
1:C:177:ASN:HD22	1:C:180:ARG:HD2	1.76	0.49
1:C:245:HIS:H	1:C:245:HIS:CD2	2.31	0.48
1:B:140:VAL:HG13	1:B:141:ARG:N	2.23	0.48
1:D:186:VAL:O	1:D:186:VAL:HG23	2.13	0.48
1:A:147:ARG:NH1	1:A:147:ARG:HB2	2.29	0.48
1:A:240:TYR:HA	1:A:245:HIS:CD2	2.49	0.48
1:C:141:ARG:HG2	2:C:426:HOH:O	2.13	0.48
1:C:238:MET:HB3	1:C:239:PRO:CD	2.44	0.48
1:B:193:GLU:HB2	1:B:202:PHE:CE2	2.49	0.47
1:B:204:ASN:ND2	2:B:353:HOH:O	2.48	0.47
1:B:123:LYS:HB3	1:B:123:LYS:HZ3	1.80	0.47
1:A:218:ILE:HD12	1:A:218:ILE:N	2.30	0.47
1:B:245:HIS:H	1:B:245:HIS:CD2	2.33	0.47
1:D:209:ASN:HB3	1:D:214:LEU:HB3	1.95	0.47
1:A:178:LYS:NZ	1:A:180:ARG:HB2	2.30	0.47
1:B:268:ALA:HB1	1:B:271:GLU:HB2	1.97	0.46
1:A:140:VAL:O	1:A:140:VAL:HG13	2.15	0.46
1:B:92:VAL:HG11	1:C:246:THR:OG1	2.15	0.46
1:B:238:MET:HB3	1:B:239:PRO:CD	2.45	0.46
1:C:209:ASN:OD1	1:C:214:LEU:HB3	2.16	0.46
1:B:191:LYS:HD3	1:B:193:GLU:OE1	2.16	0.45
1:D:205:LEU:HD22	1:D:206:SER:N	2.30	0.45
1:D:167:LYS:HG2	2:D:328:HOH:O	2.16	0.45
1:A:117:LEU:HB3	1:A:118:ASP:H	1.58	0.45
1:A:209:ASN:ND2	1:A:214:LEU:HB3	2.31	0.45
1:B:232:SER:HA	2:C:346:HOH:O	2.16	0.45
1:C:188:LYS:HD2	1:C:207:VAL:HG22	1.98	0.44
1:D:141:ARG:O	1:D:141:ARG:HG3	2.17	0.44
1:A:145:TRP:HB3	1:A:148:LYS:HD3	2.00	0.44
1:C:273:ASN:O	1:C:274:LEU:HB2	2.18	0.44
1:B:113:GLU:CG	1:B:126:ARG:HB3	2.48	0.44
1:B:140:VAL:HG13	2:B:364:HOH:O	2.17	0.44
1:A:111:SER:HA	1:A:112:PRO:HD3	1.83	0.44
1:C:186:VAL:HG23	1:C:208:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LYS:HE3	2:D:404:HOH:O	2.18	0.44
1:A:252:LYS:HD2	2:A:310:HOH:O	2.18	0.44
1:D:147:ARG:NH1	2:D:392:HOH:O	2.51	0.44
1:D:200:GLY:HA2	1:D:224:LYS:HD2	2.01	0.43
1:B:133:GLN:HG2	1:B:150:VAL:HG22	1.99	0.43
1:B:126:ARG:NH2	1:C:266:SER:N	2.63	0.43
1:B:180:ARG:HH11	1:B:180:ARG:CB	2.22	0.43
1:A:100:LYS:HA	2:A:299:HOH:O	2.19	0.42
1:A:111:SER:HB2	1:B:251:PHE:CE2	2.54	0.42
1:C:229:VAL:HG13	1:D:238:MET:SD	2.59	0.42
1:A:111:SER:HB2	1:B:251:PHE:CD2	2.55	0.42
1:A:250:SER:HB2	1:D:91:LYS:HE3	2.02	0.42
1:B:89:THR:N	1:B:90:PRO:HD2	2.33	0.42
1:D:245:HIS:CD2	1:D:245:HIS:H	2.37	0.42
1:A:105:LEU:HA	1:A:133:GLN:O	2.19	0.42
1:A:209:ASN:OD1	1:A:212:ILE:HG22	2.20	0.42
1:C:214:LEU:HD11	1:C:216:GLU:OE2	2.19	0.42
1:C:240:TYR:HA	1:C:245:HIS:CD2	2.55	0.42
1:C:185:ARG:CG	1:C:210:LYS:HB2	2.49	0.41
1:B:268:ALA:CB	1:B:271:GLU:HB2	2.49	0.41
1:C:100:LYS:HD3	1:C:100:LYS:HA	1.89	0.41
1:C:244:TRP:O	1:C:248:VAL:HB	2.20	0.41
1:C:129:MET:HB2	1:C:153:LEU:O	2.21	0.41
1:A:245:HIS:CD2	1:A:245:HIS:H	2.39	0.41
1:B:97:SER:HA	1:B:105:LEU:O	2.20	0.41
1:B:240:TYR:HA	1:B:245:HIS:CD2	2.56	0.40
1:C:135:ALA:HB2	1:C:145:TRP:CE3	2.57	0.40
1:D:271:GLU:HG3	1:D:271:GLU:O	2.21	0.40
1:A:133:GLN:HG2	1:A:150:VAL:CG1	2.43	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	164/227 (72%)	148 (90%)	12 (7%)	4 (2%)	6	4
1	B	166/227 (73%)	151 (91%)	13 (8%)	2 (1%)	13	14
1	C	178/227 (78%)	163 (92%)	9 (5%)	6 (3%)	3	2
1	D	167/227 (74%)	155 (93%)	10 (6%)	2 (1%)	13	14
All	All	675/908 (74%)	617 (91%)	44 (6%)	14 (2%)	7	5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	ASN
1	A	118	ASP
1	A	138	ALA
1	B	90	PRO
1	B	181	SER
1	C	185	ARG
1	C	212	ILE
1	D	268	ALA
1	A	181	SER
1	C	118	ASP
1	C	178	LYS
1	D	140	VAL
1	A	119	SER
1	C	176	PRO

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	144/194 (74%)	138 (96%)	6 (4%)	30	42
1	B	147/194 (76%)	140 (95%)	7 (5%)	25	36
1	C	158/194 (81%)	155 (98%)	3 (2%)	57	73
1	D	147/194 (76%)	138 (94%)	9 (6%)	18	25
All	All	596/776 (77%)	571 (96%)	25 (4%)	30	42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	147	ARG
1	A	216	GLU
1	A	230	LEU
1	A	237	VAL
1	A	238	MET
1	B	102	LYS
1	B	153	LEU
1	B	168	ASP
1	B	180	ARG
1	B	195	LEU
1	B	209	ASN
1	B	271	GLU
1	C	209	ASN
1	C	248	VAL
1	C	252	LYS
1	D	97	SER
1	D	100	LYS
1	D	141	ARG
1	D	178	LYS
1	D	197	ASP
1	D	204	ASN
1	D	205	LEU
1	D	222	VAL
1	D	237	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	208	GLN
1	A	245	HIS
1	B	209	ASN
1	B	213	ASN
1	B	245	HIS
1	C	174	HIS
1	C	245	HIS
1	D	133	GLN
1	D	142	GLN
1	D	149	GLN
1	D	174	HIS

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Mol	Chain	Res	Type
1	D	204	ASN
1	D	208	GLN
1	D	217	ASN
1	D	245	HIS
1	D	249	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 monosaccharides 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	166/227 (73%)	1.13	31 (18%) 1 1	32, 53, 101, 127	0
1	B	170/227 (74%)	0.84	21 (12%) 4 5	33, 52, 83, 95	4 (2%)
1	C	182/227 (80%)	1.10	34 (18%) 1 1	30, 48, 97, 124	0
1	D	171/227 (75%)	0.91	17 (9%) 7 10	29, 47, 85, 92	5 (2%)
All	All	689/908 (75%)	0.99	103 (14%) 2 3	29, 51, 93, 127	9 (1%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	SER	16.7
1	D	270	LEU	13.6
1	D	267	GLY	11.9
1	B	268	ALA	11.3
1	C	181	SER	11.0
1	D	269	GLU	10.3
1	B	89	THR	9.8
1	A	179	GLY	9.5
1	D	268	ALA	9.5
1	C	211	LEU	9.3
1	C	179	GLY	8.5
1	A	211	LEU	7.8
1	A	140	VAL	7.3
1	C	180	ARG	7.3
1	D	271	GLU	7.0
1	D	89	THR	6.9
1	A	180	ARG	6.9
1	A	182	ASP	6.5
1	A	185	ARG	6.3
1	A	141	ARG	6.3
1	C	119	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	212	ILE	6.2
1	C	182	ASP	6.1
1	B	140	VAL	6.0
1	B	270	LEU	5.9
1	C	267	GLY	5.8
1	A	89	THR	5.8
1	C	185	ARG	5.6
1	A	212	ILE	5.5
1	D	140	VAL	5.2
1	B	271	GLU	5.2
1	B	269	GLU	5.2
1	A	120	GLY	5.0
1	C	184	GLY	4.9
1	A	183	GLU	4.7
1	D	254	GLU	4.6
1	B	118	ASP	4.6
1	C	120	GLY	4.6
1	A	213	ASN	4.4
1	C	177	ASN	4.2
1	C	254	GLU	4.2
1	B	90	PRO	4.0
1	C	209	ASN	3.9
1	A	119	SER	3.8
1	B	231	VAL	3.7
1	A	178	LYS	3.6
1	D	197	ASP	3.4
1	C	213	ASN	3.4
1	B	120	GLY	3.4
1	C	210	LYS	3.4
1	A	147	ARG	3.4
1	B	119	SER	3.3
1	C	239	PRO	3.3
1	B	138	ALA	3.2
1	C	178	LYS	3.2
1	C	183	GLU	3.1
1	A	210	LYS	3.0
1	D	139	GLY	3.0
1	C	216	GLU	3.0
1	D	138	ALA	3.0
1	A	186	VAL	2.9
1	C	115	SER	2.9
1	B	141	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	121	ALA	2.9
1	C	173	PHE	2.8
1	D	141	ARG	2.8
1	A	139	GLY	2.8
1	A	184	GLY	2.8
1	C	118	ASP	2.7
1	C	214	LEU	2.7
1	A	110	ARG	2.7
1	C	237	VAL	2.7
1	A	90	PRO	2.6
1	A	145	TRP	2.5
1	D	219	TYR	2.5
1	A	117	LEU	2.5
1	C	161	ILE	2.5
1	B	235	ASN	2.4
1	A	177	ASN	2.4
1	A	138	ALA	2.4
1	C	233	ALA	2.4
1	C	229	VAL	2.4
1	B	232	SER	2.4
1	C	176	PRO	2.4
1	C	252	LYS	2.3
1	B	161	ILE	2.3
1	A	215	ASP	2.3
1	D	186	VAL	2.3
1	D	180	ARG	2.3
1	C	116	PRO	2.2
1	C	236	PHE	2.2
1	A	118	ASP	2.2
1	A	175	ASP	2.2
1	B	233	ALA	2.2
1	A	214	LEU	2.1
1	B	237	VAL	2.1
1	B	254	GLU	2.1
1	B	117	LEU	2.1
1	D	241	LEU	2.1
1	C	266	SER	2.1
1	B	93	PHE	2.1
1	C	162	ILE	2.0
1	D	231	VAL	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.