



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 09:42 PM EDT

PDB ID : 5YVF  
Title : Crystal structure of BFA1  
Authors : Pu, H.; Zhang, L.; Duan, Z.K.; Peng, L.W.; Liu, L.  
Deposited on : 2017-11-25  
Resolution : 2.80 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](mailto: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>.

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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	:	2.37.1
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)	:	2.37.1

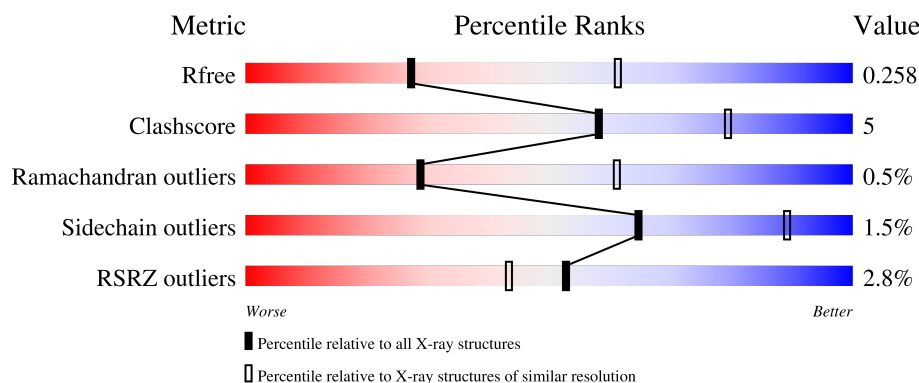
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	370	 2% 75% 11% 13%
1	B	370	 % 71% 14% 16%
1	C	370	 3% 73% 12% 14%
1	D	370	 4% 75% 10% 14%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10139 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 BFA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2545	1602	438	488	17			
1	B	312	Total	C	N	O	S	0	1	0
			2479	1570	426	466	17			
1	C	318	Total	C	N	O	S	0	1	0
			2540	1604	436	482	18			
1	D	318	Total	C	N	O	S	0	0	0
			2526	1594	435	480	17			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	expression tag	UNP A0A178VCD5
A	41	GLY	-	expression tag	UNP A0A178VCD5
A	397	LYS	-	expression tag	UNP A0A178VCD5
A	398	LEU	-	expression tag	UNP A0A178VCD5
A	399	ALA	-	expression tag	UNP A0A178VCD5
A	400	ALA	-	expression tag	UNP A0A178VCD5
A	401	ALA	-	expression tag	UNP A0A178VCD5
A	402	LEU	-	expression tag	UNP A0A178VCD5
A	403	GLU	-	expression tag	UNP A0A178VCD5
A	404	HIS	-	expression tag	UNP A0A178VCD5
A	405	HIS	-	expression tag	UNP A0A178VCD5
A	406	HIS	-	expression tag	UNP A0A178VCD5
A	407	HIS	-	expression tag	UNP A0A178VCD5
A	408	HIS	-	expression tag	UNP A0A178VCD5
A	409	HIS	-	expression tag	UNP A0A178VCD5
B	40	MET	-	expression tag	UNP A0A178VCD5
B	41	GLY	-	expression tag	UNP A0A178VCD5
B	397	LYS	-	expression tag	UNP A0A178VCD5
B	398	LEU	-	expression tag	UNP A0A178VCD5
B	399	ALA	-	expression tag	UNP A0A178VCD5
B	400	ALA	-	expression tag	UNP A0A178VCD5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	401	ALA	-	expression tag	UNP A0A178VCD5
B	402	LEU	-	expression tag	UNP A0A178VCD5
B	403	GLU	-	expression tag	UNP A0A178VCD5
B	404	HIS	-	expression tag	UNP A0A178VCD5
B	405	HIS	-	expression tag	UNP A0A178VCD5
B	406	HIS	-	expression tag	UNP A0A178VCD5
B	407	HIS	-	expression tag	UNP A0A178VCD5
B	408	HIS	-	expression tag	UNP A0A178VCD5
B	409	HIS	-	expression tag	UNP A0A178VCD5
C	40	MET	-	expression tag	UNP A0A178VCD5
C	41	GLY	-	expression tag	UNP A0A178VCD5
C	397	LYS	-	expression tag	UNP A0A178VCD5
C	398	LEU	-	expression tag	UNP A0A178VCD5
C	399	ALA	-	expression tag	UNP A0A178VCD5
C	400	ALA	-	expression tag	UNP A0A178VCD5
C	401	ALA	-	expression tag	UNP A0A178VCD5
C	402	LEU	-	expression tag	UNP A0A178VCD5
C	403	GLU	-	expression tag	UNP A0A178VCD5
C	404	HIS	-	expression tag	UNP A0A178VCD5
C	405	HIS	-	expression tag	UNP A0A178VCD5
C	406	HIS	-	expression tag	UNP A0A178VCD5
C	407	HIS	-	expression tag	UNP A0A178VCD5
C	408	HIS	-	expression tag	UNP A0A178VCD5
C	409	HIS	-	expression tag	UNP A0A178VCD5
D	40	MET	-	expression tag	UNP A0A178VCD5
D	41	GLY	-	expression tag	UNP A0A178VCD5
D	397	LYS	-	expression tag	UNP A0A178VCD5
D	398	LEU	-	expression tag	UNP A0A178VCD5
D	399	ALA	-	expression tag	UNP A0A178VCD5
D	400	ALA	-	expression tag	UNP A0A178VCD5
D	401	ALA	-	expression tag	UNP A0A178VCD5
D	402	LEU	-	expression tag	UNP A0A178VCD5
D	403	GLU	-	expression tag	UNP A0A178VCD5
D	404	HIS	-	expression tag	UNP A0A178VCD5
D	405	HIS	-	expression tag	UNP A0A178VCD5
D	406	HIS	-	expression tag	UNP A0A178VCD5
D	407	HIS	-	expression tag	UNP A0A178VCD5
D	408	HIS	-	expression tag	UNP A0A178VCD5
D	409	HIS	-	expression tag	UNP A0A178VCD5

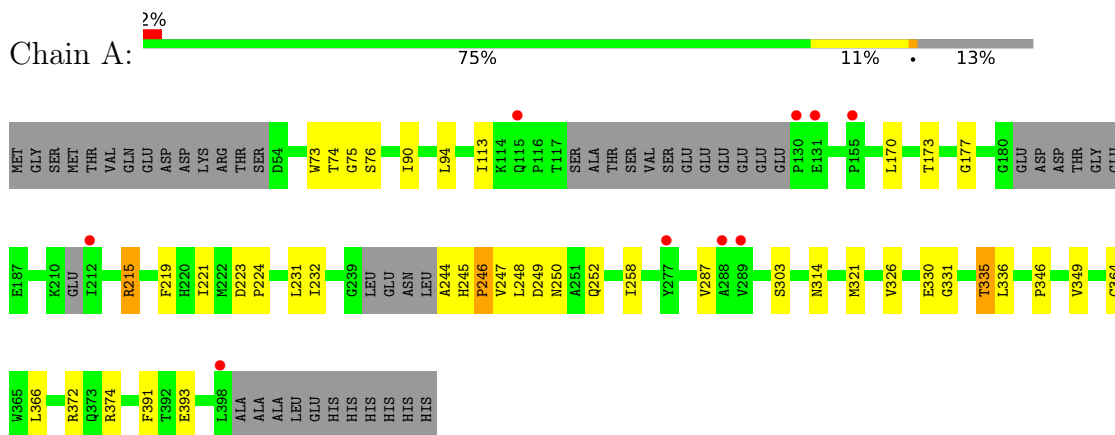
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total 11	O 11	0	0
2	B	18	Total 18	O 18	0	0
2	C	10	Total 10	O 10	0	0
2	D	10	Total 10	O 10	0	0

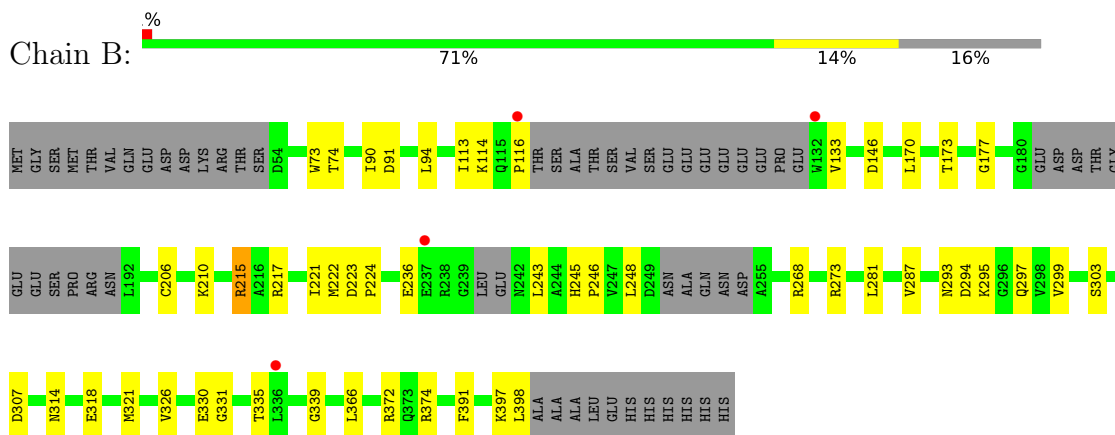
### 3 Residue-property plots

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.

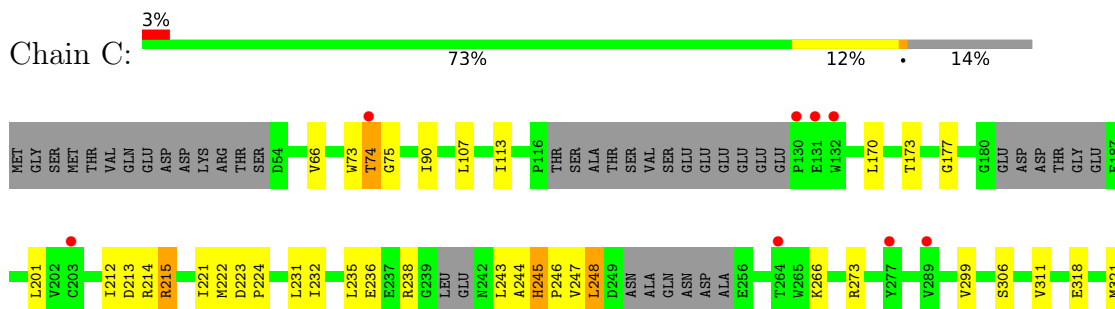
#### • Molecule 1: BFA1

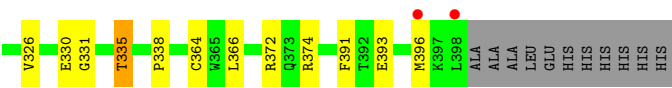


#### • Molecule 1: BFA1

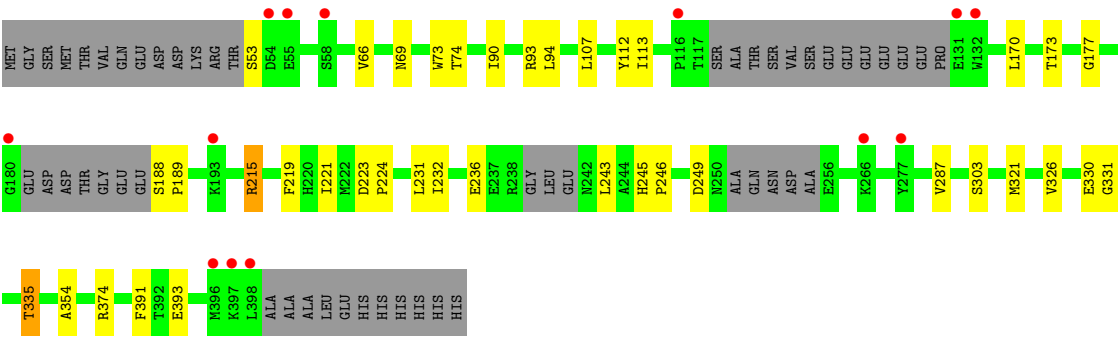


#### • Molecule 1: BFA1





● Molecule 1: BFA1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.92Å 134.63Å 149.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 2.80 46.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.73-2.80) 99.5 (46.73-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.221 , 0.261 0.220 , 0.258	Depositor DCC
$R_{free}$ test set	2006 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 14.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9415e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.32	0/2594	0.52	0/3498
1	B	0.34	0/2529	0.52	0/3405
1	C	0.29	0/2589	0.51	0/3485
1	D	0.31	0/2574	0.50	0/3468
All	All	0.32	0/10286	0.51	0/13856

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	2545	0	2483	23	0
1	B	2479	0	2450	25	0
1	C	2540	0	2506	27	1
1	D	2526	0	2486	21	1
2	A	11	0	0	0	0
2	B	18	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
All	All	10139	0	9925	95	1

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 5.

All (95) 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:374:ARG:HB2	1:A:391:PHE:HB2	1.73	0.71
1:D:73:TRP:HB2	1:D:94:LEU:HB3	1.73	0.68
1:B:374:ARG:HB2	1:B:391:PHE:HB2	1.77	0.67
1:A:321:MET:HG2	1:A:326:VAL:HG22	1.79	0.65
1:B:294:ASP:OD1	1:B:295:LYS:N	2.30	0.64
1:B:91:ASP:HB3	1:B:245:HIS:CE1	2.33	0.64
1:A:244:ALA:O	1:A:245:HIS:C	2.29	0.64
1:D:374:ARG:HB2	1:D:391:PHE:HB2	1.80	0.63
1:A:314:ASN:HB2	1:B:314:ASN:HB2	1.82	0.62
1:B:210:LYS:NZ	2:B:501:HOH:O	2.34	0.60
1:C:90:ILE:HD13	1:C:177:GLY:HA3	1.82	0.60
1:B:90:ILE:HD13	1:B:177:GLY:HA3	1.82	0.60
1:D:90:ILE:HD13	1:D:177:GLY:HA3	1.84	0.59
1:C:231:LEU:HD11	1:C:335:THR:HG21	1.85	0.59
1:C:74:THR:HG21	1:C:243:LEU:HB2	1.84	0.58
1:C:374:ARG:HB2	1:C:391:PHE:HB2	1.85	0.58
1:C:321:MET:HG2	1:C:326:VAL:HG22	1.86	0.57
1:D:321:MET:HG2	1:D:326:VAL:HG22	1.85	0.57
1:A:231:LEU:HD11	1:A:335:THR:HG21	1.85	0.57
1:A:330:GLU:N	1:A:331:GLY:HA2	2.20	0.57
1:C:330:GLU:N	1:C:331:GLY:HA2	2.20	0.57
1:B:287:VAL:HB	1:B:303:SER:HB3	1.87	0.56
1:D:223:ASP:HB2	1:D:224:PRO:HD2	1.86	0.56
1:A:73:TRP:HB2	1:A:94:LEU:HB3	1.86	0.56
1:B:330:GLU:N	1:B:331:GLY:HA2	2.19	0.56
1:B:248:LEU:HD22	1:B:339:GLY:HA3	1.87	0.55
1:B:273:ARG:HB2	1:B:281:LEU:HD21	1.89	0.55
1:C:306:SER:HB3	1:C:311:VAL:HG22	1.89	0.55
1:B:321:MET:HG2	1:B:326:VAL:HG22	1.88	0.55
1:D:330:GLU:N	1:D:331:GLY:HA2	2.22	0.54
1:B:299:VAL:HG22	1:B:318:GLU:HG2	1.89	0.54
1:A:223:ASP:HB2	1:A:224:PRO:HD2	1.90	0.53
1:D:231:LEU:HD11	1:D:335:THR:HG21	1.89	0.53
1:B:113:ILE:HD13	1:B:173:THR:HA	1.91	0.53
1:D:66:VAL:HG22	1:D:107:LEU:HB2	1.91	0.53
1:B:268:ARG:NH2	1:B:307:ASP:OD2	2.42	0.52
1:C:299:VAL:HG22	1:C:318:GLU:HG2	1.90	0.52
1:A:90:ILE:HD13	1:A:177:GLY:HA3	1.90	0.52
1:B:116:PRO:HB3	1:B:133:VAL:HB	1.90	0.52
1:C:247:VAL:O	1:C:248:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ILE:HD13	1:A:173:THR:HA	1.93	0.51
1:C:170:LEU:HD22	1:C:232:ILE:HD13	1.93	0.51
1:D:113:ILE:HD13	1:D:173:THR:HA	1.94	0.49
1:D:287:VAL:HB	1:D:303:SER:HB3	1.92	0.49
1:D:74:THR:HG21	1:D:243:LEU:HB2	1.94	0.49
1:C:266:LYS:HE3	1:C:396[B]:MET:SD	2.53	0.49
1:D:215:ARG:NH1	1:D:236:GLU:OE1	2.44	0.49
1:C:212:ILE:HG13	1:C:214:ARG:HG2	1.95	0.48
1:C:223:ASP:HB2	1:C:224:PRO:HD2	1.95	0.48
1:C:231:LEU:CD1	1:C:335:THR:HG21	2.44	0.48
1:D:170:LEU:HD22	1:D:232:ILE:HD13	1.96	0.48
1:A:366:LEU:HB3	1:A:372:ARG:HB3	1.96	0.47
1:C:75:GLY:HA3	1:C:236:GLU:HG2	1.97	0.47
1:C:73:TRP:CZ3	1:C:215:ARG:HG2	2.50	0.46
1:C:244:ALA:O	1:C:245:HIS:HB2	2.15	0.46
1:A:287:VAL:HB	1:A:303:SER:HB3	1.97	0.46
1:C:113:ILE:HD13	1:C:173:THR:HA	1.96	0.46
1:C:374:ARG:HD3	1:C:393:GLU:OE1	2.16	0.46
1:A:248:LEU:O	1:A:250:ASN:N	2.48	0.46
1:B:397:LYS:O	1:B:398:LEU:HB3	2.16	0.45
1:D:245:HIS:HA	1:D:246:PRO:HD3	1.81	0.45
1:C:245:HIS:HA	1:C:246:PRO:HD3	1.75	0.45
1:A:170:LEU:HD13	1:A:221:ILE:HD11	1.99	0.44
1:B:73:TRP:HB2	1:B:94:LEU:HB3	1.98	0.44
1:A:374:ARG:HD3	1:A:393:GLU:OE1	2.18	0.44
1:A:75:GLY:HA2	1:A:246:PRO:HD2	1.99	0.43
1:A:247:VAL:HG12	1:A:248:LEU:O	2.18	0.43
1:B:170:LEU:HD13	1:B:221:ILE:HD11	2.00	0.43
1:C:364:CYS:HB2	1:C:374:ARG:HG2	2.00	0.43
1:C:170:LEU:HD13	1:C:221:ILE:HD11	2.00	0.43
1:A:364:CYS:HB2	1:A:374:ARG:HG2	2.00	0.43
1:C:201:LEU:HB3	1:C:222:MET:HG2	2.01	0.43
1:B:215:ARG:NH1	1:B:236:GLU:OE1	2.42	0.43
1:A:346:PRO:HG2	1:A:349:VAL:HG22	2.00	0.42
1:B:74:THR:HG21	1:B:243:LEU:H	1.84	0.42
1:A:258:ILE:HB	1:A:336:LEU:HD13	2.01	0.42
1:D:188:SER:HA	1:D:189:PRO:HD3	1.79	0.42
1:A:366:LEU:HA	1:A:372:ARG:HA	2.01	0.42
1:D:69:ASN:OD1	1:D:215:ARG:NH2	2.52	0.42
1:D:219:PHE:HB2	1:D:232:ILE:HB	2.01	0.42
1:A:73:TRP:CZ3	1:A:215:ARG:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:CYS:SG	1:B:217:ARG:HG2	2.60	0.42
1:B:223:ASP:HB2	1:B:224:PRO:HD2	2.01	0.42
1:C:366:LEU:HA	1:C:372:ARG:HA	2.02	0.42
1:C:248:LEU:HD13	1:C:338:PRO:HB2	2.02	0.42
1:D:374:ARG:HD3	1:D:393:GLU:OE1	2.20	0.42
1:D:93:ARG:HB2	1:D:112:TYR:HB2	2.02	0.42
1:A:219:PHE:HB2	1:A:232:ILE:HB	2.02	0.41
1:D:170:LEU:HD13	1:D:221:ILE:HD11	2.02	0.41
1:C:66:VAL:HG22	1:C:107:LEU:HB2	2.02	0.41
1:B:366:LEU:HB3	1:B:372:ARG:HB3	2.03	0.41
1:B:91:ASP:HB2	1:B:114:LYS:HD3	2.03	0.40
1:B:245:HIS:HA	1:B:246:PRO:HD3	1.74	0.40
1:C:213:ASP:OD2	1:C:238:ARG:HB3	2.21	0.40
1:D:170:LEU:CD1	1:D:221:ILE:HD11	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:NH1	1:D:354:ALA:O[4_555]	2.15	0.05

## 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	312/370 (84%)	301 (96%)	9 (3%)	2 (1%)	25	56
1	B	303/370 (82%)	291 (96%)	11 (4%)	1 (0%)	41	72
1	C	309/370 (84%)	299 (97%)	8 (3%)	2 (1%)	25	56
1	D	308/370 (83%)	299 (97%)	8 (3%)	1 (0%)	41	72
All	All	1232/1480 (83%)	1190 (97%)	36 (3%)	6 (0%)	29	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ASP
1	C	248	LEU
1	C	245	HIS
1	D	249	ASP
1	B	293	ASN
1	A	246	PRO

### 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	281/327 (86%)	276 (98%)	5 (2%)	59	86
1	B	273/327 (84%)	268 (98%)	5 (2%)	59	86
1	C	283/327 (86%)	279 (99%)	4 (1%)	67	90
1	D	281/327 (86%)	278 (99%)	3 (1%)	73	92
All	All	1118/1308 (86%)	1101 (98%)	17 (2%)	65	89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	76	SER
1	A	215	ARG
1	A	252	GLN
1	A	335	THR
1	B	146	ASP
1	B	215	ARG
1	B	222	MET
1	B	297	GLN
1	B	335	THR
1	C	74	THR
1	C	215	ARG
1	C	235	LEU
1	C	335	THR

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Mol	Chain	Res	Type
1	D	53	SER
1	D	215	ARG
1	D	335	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides 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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	322/370 (87%)	-0.02	9 (2%)	53	43	12, 25, 65, 94	0
1	B	312/370 (84%)	-0.08	4 (1%)	77	72	11, 24, 57, 80	0
1	C	318/370 (85%)	0.04	10 (3%)	49	39	13, 27, 64, 87	0
1	D	318/370 (85%)	0.08	13 (4%)	37	27	14, 29, 65, 91	0
All	All	1270/1480 (85%)	0.01	36 (2%)	53	43	11, 26, 63, 94	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	398	LEU	5.2
1	C	132	TRP	4.7
1	D	398	LEU	3.8
1	B	116	PRO	3.8
1	A	289	VAL	3.6
1	D	54	ASP	3.6
1	A	212	ILE	3.5
1	A	398	LEU	3.3
1	C	130	PRO	3.2
1	A	288	ALA	3.2
1	B	237	GLU	3.1
1	D	396	MET	3.1
1	D	132	TRP	2.9
1	D	58	SER	2.8
1	C	396[A]	MET	2.8
1	B	132	TRP	2.7
1	D	180	GLY	2.7
1	D	116	PRO	2.7
1	C	131	GLU	2.6
1	D	193	LYS	2.5
1	C	277	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	277	TYR	2.5
1	A	277	TYR	2.4
1	A	155	PRO	2.4
1	D	131	GLU	2.3
1	A	131	GLU	2.3
1	D	266	LYS	2.3
1	A	115	GLN	2.3
1	C	264	THR	2.2
1	C	203	CYS	2.2
1	D	55	GLU	2.2
1	B	336	LEU	2.2
1	D	397	LYS	2.2
1	C	74	THR	2.1
1	A	130	PRO	2.1
1	C	289	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.