



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:43 AM GMT

PDB ID : 2E2L  
Title : Helicobacter pylori formamidase AmiF contains a fine-tuned cysteine-glutamate-lysine catalytic triad  
Authors : Wang, W.C.; Hung, C.L.  
Deposited on : 2006-11-14  
Resolution : 2.29 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
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

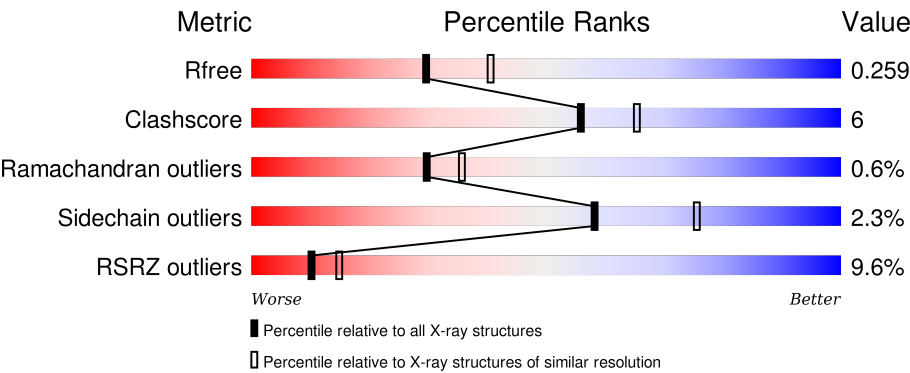
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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 <sub>free</sub>	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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 <=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	334	<div><div>7%</div><div>81%13%5%</div></div>
1	B	334	<div><div>11%</div><div>79%15%5%</div></div>
1	C	334	<div><div>7%</div><div>79%14%5%</div></div>
1	D	334	<div><div>7%</div><div>82%12%5%</div></div>
1	E	334	<div><div>10%</div><div>83%10%5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ARF	A	1335	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15751 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.

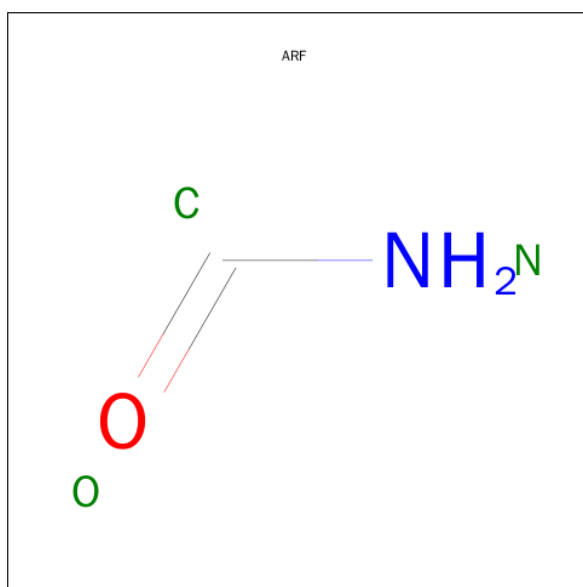
- Molecule 1 is a protein called Formamidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			
1	B	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			
1	C	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			
1	D	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			
1	E	316	Total	C	N	O	S	0	0	0
			2492	1604	417	460	11			
1	F	317	Total	C	N	O	S	0	0	0
			2503	1610	421	461	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	SER	CYS	ENGINEERED	UNP O25836
B	166	SER	CYS	ENGINEERED	UNP O25836
C	166	SER	CYS	ENGINEERED	UNP O25836
D	166	SER	CYS	ENGINEERED	UNP O25836
E	166	SER	CYS	ENGINEERED	UNP O25836
F	166	SER	CYS	ENGINEERED	UNP O25836

- Molecule 2 is FORMAMIDE (three-letter code: ARF) (formula: CH<sub>3</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			3	1	1	1		
2	C	1	Total	C	N	O	0	0
			3	1	1	1		
2	F	1	Total	C	N	O	0	0
			3	1	1	1		

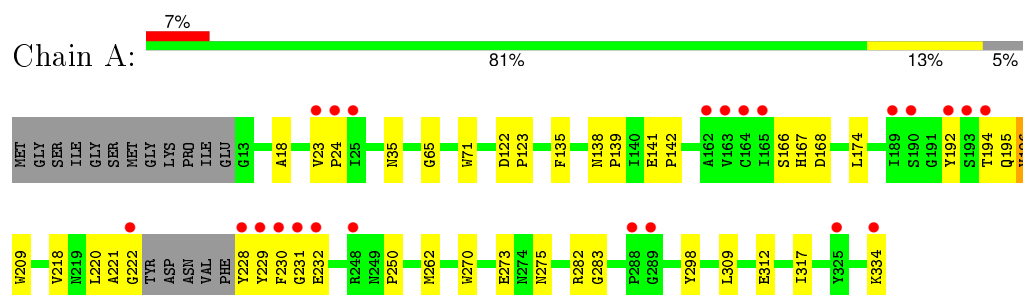
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		
3	B	131	Total	O	0	0
			131	131		
3	C	143	Total	O	0	0
			143	143		
3	D	102	Total	O	0	0
			102	102		
3	E	114	Total	O	0	0
			114	114		
3	F	112	Total	O	0	0
			112	112		

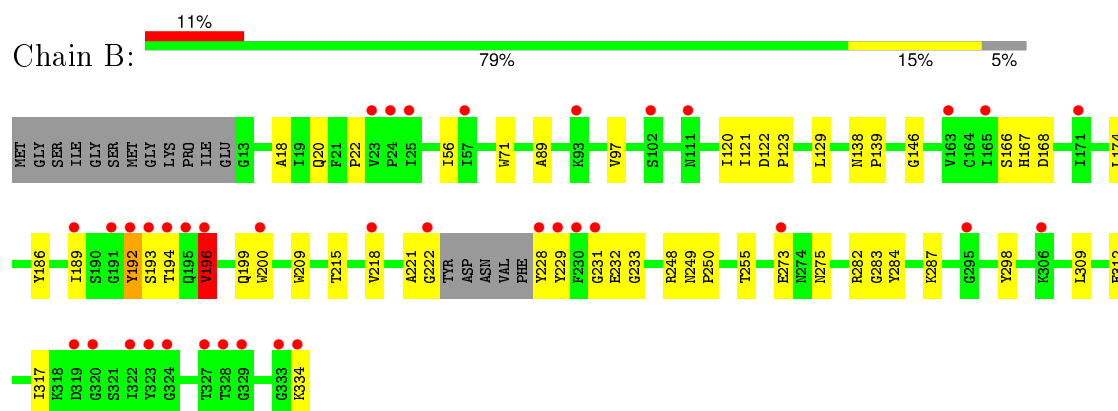
### 3 Residue-property plots [i](#)

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.

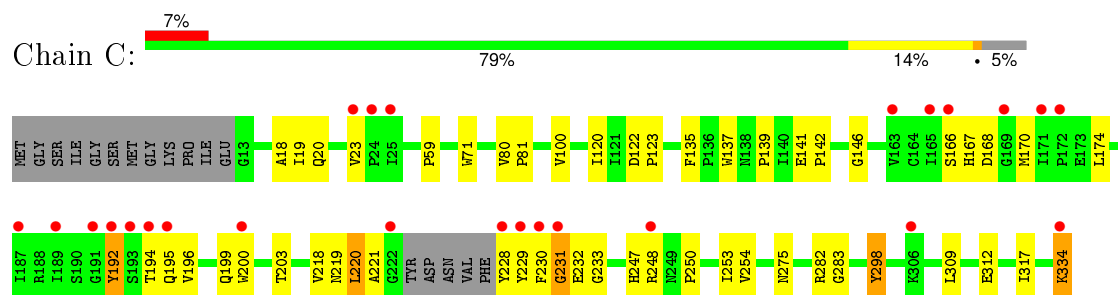
#### • Molecule 1: Formamidase



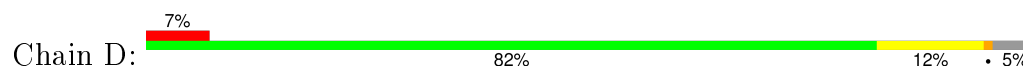
#### • Molecule 1: Formamidase

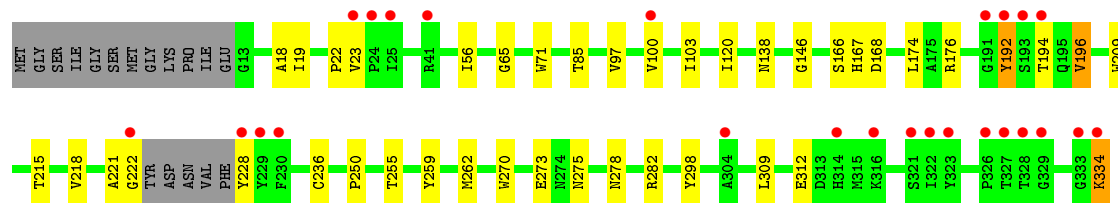


#### • Molecule 1: Formamidase

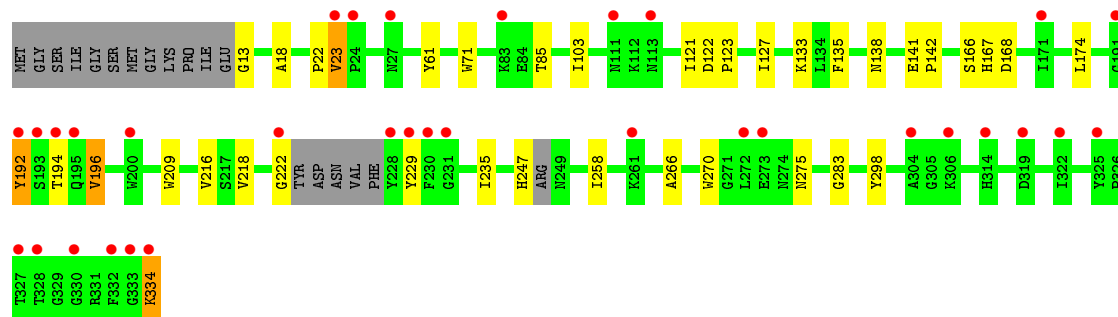
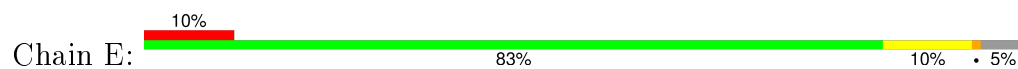


#### • Molecule 1: Formamidase

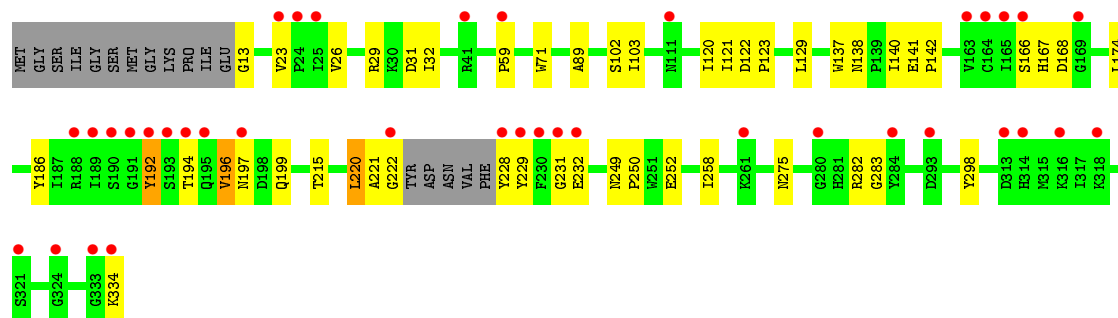
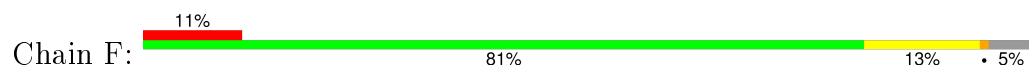




• Molecule 1: Formamidase



• Molecule 1: Formamidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.09Å 151.79Å 89.08Å 90.00° 114.99° 90.00°	Depositor
Resolution (Å)	30.00 – 2.29 29.62 – 2.29	Depositor EDS
% Data completeness (in resolution range)	90.9 (30.00-2.29) 90.9 (29.62-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.253 , 0.285 0.252 , 0.259	Depositor DCC
$R_{free}$ test set	4091 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.8	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 81861 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ARF

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	0.33	0/2574	0.50	0/3498
1	B	0.33	0/2574	0.48	0/3498
1	C	0.33	0/2574	0.50	0/3498
1	D	0.33	0/2574	0.49	0/3498
1	E	0.33	0/2562	0.48	0/3481
1	F	0.33	0/2574	0.48	0/3498
All	All	0.33	0/15432	0.49	0/20971

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	2503	0	2442	43	0
1	B	2503	0	2442	47	0
1	C	2503	0	2442	48	0
1	D	2503	0	2442	41	0
1	E	2492	0	2428	24	0
1	F	2503	0	2442	30	0
2	A	3	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	3	1	0
2	F	3	0	3	0	0
3	A	133	0	0	3	0
3	B	131	0	0	1	0
3	C	143	0	0	1	0
3	D	102	0	0	2	0
3	E	114	0	0	1	0
3	F	112	0	0	0	0
All	All	15751	0	14647	185	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 6.

All (185) 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:C:170:MET:CE	1:D:209:TRP:HE1	1.66	1.08
1:C:170:MET:HE2	1:D:209:TRP:HE1	1.24	1.00
1:A:192:TYR:HD2	2:A:1335:ARF:HN2	1.27	0.81
1:C:170:MET:HE2	1:D:209:TRP:NE1	1.96	0.80
1:C:170:MET:CE	1:D:209:TRP:NE1	2.47	0.77
1:C:282:ARG:NH2	1:D:146:GLY:O	2.20	0.74
1:C:219:ASN:HB3	1:C:231:GLY:HA2	1.68	0.73
1:A:275:ASN:HD22	1:B:167:HIS:HE1	1.37	0.71
1:C:334:LYS:H	1:C:334:LYS:HD2	1.58	0.69
1:C:275:ASN:ND2	1:D:167:HIS:HE1	1.91	0.68
1:C:275:ASN:HD22	1:D:167:HIS:HE1	1.38	0.67
1:A:283:GLY:HA2	1:B:138:ASN:HD21	1.58	0.67
1:D:23:VAL:HG21	1:D:65:GLY:HA2	1.77	0.66
1:B:200:TRP:HZ3	1:B:232:GLU:O	1.78	0.65
1:A:309:LEU:HB2	1:A:312:GLU:HG3	1.79	0.65
1:C:170:MET:HE3	1:C:203:THR:HG21	1.78	0.65
1:E:138:ASN:HD21	1:F:283:GLY:HA2	1.61	0.65
1:A:282:ARG:NH2	1:B:146:GLY:O	2.24	0.65
1:F:196:VAL:HG12	1:F:199:GLN:HB2	1.80	0.64
1:B:192:TYR:H	1:B:192:TYR:HD2	1.45	0.62
1:E:85:THR:HG22	1:E:103:ILE:HD13	1.81	0.61
1:E:192:TYR:N	1:E:192:TYR:HD2	1.99	0.60
1:A:230:PHE:HB2	3:A:1461:HOH:O	2.00	0.60
1:A:168:ASP:HB3	1:A:174:LEU:HD23	1.83	0.60
1:B:192:TYR:O	1:B:194:THR:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLY:HA3	1:A:228:TYR:HB3	1.83	0.59
1:A:229:TYR:CD2	1:D:250:PRO:O	2.56	0.58
1:C:200:TRP:HZ3	1:C:232:GLU:O	1.86	0.58
1:A:275:ASN:ND2	1:B:167:HIS:HE1	1.99	0.58
1:A:192:TYR:HD2	2:A:1335:ARF:N	1.99	0.58
1:F:59:PRO:HB2	1:F:220:LEU:HD13	1.85	0.58
1:A:23:VAL:N	1:A:222:GLY:O	2.36	0.58
1:A:275:ASN:HD22	1:B:167:HIS:CE1	2.20	0.57
1:E:192:TYR:N	1:E:192:TYR:CD2	2.71	0.57
1:C:167:HIS:HE1	1:D:275:ASN:ND2	2.03	0.57
1:E:266:ALA:O	1:E:270:TRP:HB2	2.05	0.56
1:A:135:PHE:CE1	1:B:282:ARG:HG2	2.40	0.56
1:C:146:GLY:O	1:D:282:ARG:NH2	2.33	0.56
1:B:309:LEU:HB2	1:B:312:GLU:HG3	1.87	0.56
1:A:195:GLN:HG3	1:D:255:THR:OG1	2.06	0.56
1:A:250:PRO:O	1:E:229:TYR:CD2	2.59	0.55
1:F:194:THR:C	1:F:196:VAL:H	2.10	0.55
1:B:209:TRP:HH2	1:B:273:GLU:HB3	1.72	0.55
1:C:199:GLN:HG2	1:D:209:TRP:CD2	2.42	0.55
1:D:194:THR:C	1:D:196:VAL:H	2.09	0.54
1:B:18:ALA:HB1	1:B:218:VAL:HB	1.89	0.54
1:E:283:GLY:HA2	1:F:138:ASN:HD21	1.71	0.54
1:C:283:GLY:HA2	1:D:138:ASN:HD21	1.73	0.54
1:E:247:HIS:C	3:E:447:HOH:O	2.45	0.54
1:B:250:PRO:O	1:C:229:TYR:CD2	2.61	0.54
1:C:250:PRO:O	1:F:229:TYR:CD2	2.61	0.54
1:A:275:ASN:ND2	1:B:167:HIS:CE1	2.75	0.53
1:D:192:TYR:CD2	1:D:192:TYR:N	2.75	0.53
1:A:270:TRP:CE3	1:A:273:GLU:HB2	2.44	0.53
1:B:20:GLN:NE2	1:B:233:GLY:H	2.07	0.53
1:A:221:ALA:HA	1:A:231:GLY:CA	2.39	0.52
1:F:231:GLY:O	1:F:232:GLU:HG2	2.10	0.52
1:C:167:HIS:CE1	1:D:275:ASN:ND2	2.77	0.52
1:C:194:THR:C	1:C:196:VAL:H	2.12	0.51
1:D:18:ALA:HB1	1:D:218:VAL:HB	1.93	0.51
1:A:138:ASN:HD21	1:B:283:GLY:HA2	1.75	0.51
1:B:20:GLN:HE21	1:B:233:GLY:H	1.59	0.51
1:A:192:TYR:HA	3:A:1464:HOH:O	2.11	0.51
1:F:222:GLY:HA2	1:F:228:TYR:HA	1.92	0.50
1:F:168:ASP:HB3	1:F:174:LEU:HD23	1.94	0.50
1:C:275:ASN:ND2	1:D:167:HIS:CE1	2.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ALA:HB1	1:C:218:VAL:HB	1.92	0.50
1:D:221:ALA:HB3	1:D:250:PRO:HA	1.93	0.50
1:D:22:PRO:HA	1:D:222:GLY:H	1.76	0.50
1:D:19:ILE:HD11	1:D:56:ILE:HG23	1.92	0.50
1:A:220:LEU:O	1:A:231:GLY:HA2	2.12	0.49
1:A:24:PRO:HA	1:A:228:TYR:CE1	2.48	0.49
1:E:122:ASP:HB2	1:E:123:PRO:CD	2.43	0.49
1:C:192:TYR:HD2	1:C:192:TYR:H	1.60	0.49
1:D:282:ARG:HG3	3:D:387:HOH:O	2.13	0.49
1:F:221:ALA:HA	1:F:231:GLY:N	2.28	0.49
1:D:22:PRO:HB3	1:D:250:PRO:HB3	1.94	0.48
1:B:196:VAL:HG12	1:B:199:GLN:HB2	1.96	0.48
1:C:309:LEU:HB2	1:C:312:GLU:HG3	1.95	0.48
1:C:135:PHE:CE1	1:D:282:ARG:HG2	2.49	0.48
1:B:222:GLY:HA2	1:B:228:TYR:HA	1.96	0.48
1:C:100:VAL:HG22	1:C:120:ILE:HG12	1.95	0.48
1:D:309:LEU:HB2	1:D:312:GLU:HG3	1.94	0.48
1:D:270:TRP:CE3	1:D:273:GLU:HB2	2.49	0.48
1:A:228:TYR:O	1:A:250:PRO:HG3	2.14	0.48
1:B:228:TYR:O	1:B:250:PRO:HG3	2.14	0.47
1:B:209:TRP:CH2	1:B:273:GLU:HB3	2.49	0.47
1:B:168:ASP:HB3	1:B:174:LEU:HD23	1.97	0.47
1:A:18:ALA:HB1	1:A:218:VAL:HB	1.95	0.47
1:F:102:SER:O	1:F:103:ILE:HG13	2.14	0.47
1:E:135:PHE:CE1	1:F:282:ARG:HG2	2.49	0.47
1:B:249:ASN:HB3	1:C:229:TYR:CG	2.49	0.47
1:C:192:TYR:CD2	1:C:192:TYR:N	2.81	0.47
1:D:23:VAL:CG2	1:D:65:GLY:HA2	2.42	0.47
1:C:122:ASP:HB2	1:C:123:PRO:CD	2.45	0.47
1:A:122:ASP:HB2	1:A:123:PRO:CD	2.45	0.47
1:E:216:VAL:HG13	1:E:235:ILE:HG12	1.96	0.46
1:E:275:ASN:ND2	1:F:167:HIS:CE1	2.84	0.46
1:A:167:HIS:CE1	1:B:275:ASN:HD22	2.33	0.46
1:C:221:ALA:HA	1:C:231:GLY:H	1.80	0.46
1:E:334:LYS:HD2	1:E:334:LYS:H	1.80	0.46
1:B:194:THR:C	1:B:196:VAL:H	2.19	0.46
1:F:221:ALA:HB3	1:F:250:PRO:HA	1.98	0.46
1:D:215:THR:OG1	1:D:236:CYS:HB2	2.16	0.46
1:C:221:ALA:HB3	1:C:250:PRO:HA	1.98	0.46
1:E:168:ASP:HB3	1:E:174:LEU:HD23	1.98	0.46
1:E:18:ALA:HB1	1:E:218:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TYR:HA	1:B:287:LYS:O	2.16	0.45
1:B:282:ARG:HG3	3:B:369:HOH:O	2.16	0.45
1:B:89:ALA:HA	1:B:121:ILE:HG21	1.99	0.45
1:F:89:ALA:HA	1:F:121:ILE:HG21	1.99	0.45
1:D:209:TRP:HH2	1:D:273:GLU:HB3	1.82	0.45
1:E:192:TYR:H	1:E:192:TYR:HD2	1.64	0.45
1:A:270:TRP:HE3	1:A:273:GLU:HB2	1.82	0.44
1:A:35:ASN:ND2	3:A:1376:HOH:O	2.50	0.44
1:C:221:ALA:O	1:C:228:TYR:C	2.56	0.44
1:F:122:ASP:HB2	1:F:123:PRO:CD	2.47	0.44
1:D:100:VAL:HG22	1:D:120:ILE:HG12	2.00	0.44
1:A:200:TRP:CZ3	1:A:232:GLU:HB3	2.53	0.44
1:D:194:THR:C	1:D:196:VAL:N	2.70	0.44
1:F:29:ARG:HA	1:F:32:ILE:HD12	1.98	0.44
1:B:255:THR:OG1	1:C:195:GLN:HG3	2.18	0.44
1:A:222:GLY:CA	1:A:228:TYR:HB3	2.45	0.44
1:B:186:TYR:HB3	1:B:215:THR:HG22	2.00	0.44
1:B:229:TYR:CG	1:F:249:ASN:HB3	2.52	0.43
1:C:167:HIS:HE1	1:D:275:ASN:HD22	1.64	0.43
1:F:120:ILE:HD12	1:F:129:LEU:HD13	1.99	0.43
1:F:13:GLY:HA3	1:F:258:ILE:O	2.19	0.43
1:D:85:THR:HG22	1:D:103:ILE:HD13	2.00	0.43
1:A:167:HIS:CE1	1:B:275:ASN:ND2	2.86	0.43
1:B:248:ARG:NH1	1:F:252:GLU:OE2	2.51	0.43
1:E:121:ILE:HG12	1:E:127:ILE:HG12	2.01	0.43
1:B:221:ALA:HA	1:B:231:GLY:H	1.84	0.43
1:F:141:GLU:HA	1:F:142:PRO:HD3	1.85	0.43
1:B:229:TYR:CD2	1:F:250:PRO:O	2.72	0.43
1:C:233:GLY:HA3	1:C:254:VAL:HG21	2.00	0.43
1:D:168:ASP:HB3	1:D:174:LEU:HD23	2.00	0.43
1:A:221:ALA:HA	1:A:231:GLY:HA3	1.99	0.43
1:B:122:ASP:HB2	1:B:123:PRO:CD	2.48	0.43
1:B:189:ILE:O	1:B:189:ILE:HG13	2.19	0.42
1:E:209:TRP:CD2	1:F:199:GLN:HG2	2.54	0.42
1:A:209:TRP:CD2	1:B:199:GLN:HG2	2.54	0.42
1:A:139:PRO:HG3	1:A:317:ILE:HG21	2.01	0.42
1:F:137:TRP:O	1:F:140:ILE:HG22	2.19	0.42
1:C:59:PRO:HB2	1:C:220:LEU:HD13	2.02	0.42
1:F:186:TYR:HB3	1:F:215:THR:HG22	2.02	0.42
1:F:192:TYR:O	1:F:194:THR:N	2.44	0.42
1:E:167:HIS:CE1	1:F:275:ASN:ND2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLU:HA	1:C:142:PRO:HD3	1.82	0.42
1:C:168:ASP:HB3	1:C:174:LEU:HD23	2.02	0.42
1:B:192:TYR:N	1:B:192:TYR:CD2	2.85	0.42
1:D:56:ILE:HD12	1:D:97:VAL:HG21	2.02	0.42
1:A:23:VAL:HG21	1:A:65:GLY:HA2	2.01	0.42
1:C:192:TYR:HA	3:C:2472:HOH:O	2.19	0.41
1:C:139:PRO:HG3	1:C:317:ILE:HG21	2.01	0.41
1:E:13:GLY:HA3	1:E:258:ILE:O	2.20	0.41
1:E:194:THR:C	1:E:196:VAL:H	2.22	0.41
1:E:141:GLU:HA	1:E:142:PRO:HD3	1.86	0.41
1:C:194:THR:HB	1:C:230:PHE:CD1	2.55	0.41
1:D:334:LYS:H	1:D:334:LYS:HD2	1.85	0.41
1:B:139:PRO:HG3	1:B:317:ILE:HG21	2.02	0.41
1:A:199:GLN:HG2	1:B:209:TRP:CD2	2.55	0.41
1:B:249:ASN:ND2	1:C:248:ARG:HB2	2.36	0.41
1:C:80:VAL:HA	1:C:81:PRO:HA	1.91	0.41
1:A:194:THR:C	1:A:196:VAL:H	2.24	0.41
1:C:19:ILE:HG13	1:C:253:ILE:HD12	2.02	0.41
1:D:278:ASN:ND2	3:D:339:HOH:O	2.54	0.41
1:C:20:GLN:NE2	1:C:233:GLY:H	2.18	0.41
1:C:170:MET:CE	1:C:203:THR:HG21	2.50	0.41
1:A:283:GLY:CA	1:B:138:ASN:HD21	2.30	0.41
1:B:120:ILE:HD12	1:B:129:LEU:HD13	2.03	0.41
1:A:141:GLU:HA	1:A:142:PRO:HD3	1.85	0.41
1:C:137:TRP:CE3	2:C:2335:ARF:H	2.56	0.41
1:A:221:ALA:HB3	1:A:250:PRO:HA	2.03	0.41
1:E:23:VAL:HG21	1:E:61:TYR:O	2.21	0.41
1:C:231:GLY:O	1:C:247:HIS:O	2.39	0.40
1:F:26:VAL:HG13	1:F:31:ASP:HB2	2.02	0.40
1:E:22:PRO:HA	1:E:222:GLY:HA3	2.03	0.40
1:D:259:TYR:HB3	1:D:262:MET:HE3	2.03	0.40
1:F:23:VAL:N	1:F:222:GLY:O	2.54	0.40
1:C:298:TYR:CE1	1:D:176:ARG:HG2	2.56	0.40
1:D:23:VAL:HG12	1:D:222:GLY:C	2.42	0.40
1:A:138:ASN:HD21	1:B:283:GLY:CA	2.34	0.40
1:A:167:HIS:HE1	1:B:275:ASN:ND2	2.20	0.40
1:B:56:ILE:HD12	1:B:97:VAL:HG21	2.04	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	313/334 (94%)	300 (96%)	12 (4%)	1 (0%)	46	57
1	B	313/334 (94%)	298 (95%)	11 (4%)	4 (1%)	15	15
1	C	313/334 (94%)	298 (95%)	13 (4%)	2 (1%)	30	36
1	D	313/334 (94%)	302 (96%)	10 (3%)	1 (0%)	46	57
1	E	310/334 (93%)	299 (96%)	9 (3%)	2 (1%)	30	36
1	F	313/334 (94%)	299 (96%)	13 (4%)	1 (0%)	46	57
All	All	1875/2004 (94%)	1796 (96%)	68 (4%)	11 (1%)	30	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	B	193	SER
1	C	231	GLY
1	E	166	SER
1	F	166	SER
1	B	166	SER
1	C	166	SER
1	D	166	SER
1	E	133	LYS
1	B	22	PRO
1	B	196	VAL

### 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	263/277 (95%)	257 (98%)	6 (2%)	58	75
1	B	263/277 (95%)	258 (98%)	5 (2%)	65	81
1	C	263/277 (95%)	257 (98%)	6 (2%)	58	75
1	D	263/277 (95%)	257 (98%)	6 (2%)	58	75
1	E	262/277 (95%)	256 (98%)	6 (2%)	58	75
1	F	263/277 (95%)	256 (97%)	7 (3%)	52	70
All	All	1577/1662 (95%)	1541 (98%)	36 (2%)	58	75

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TRP
1	A	196	VAL
1	A	197	ASN
1	A	262	MET
1	A	298	TYR
1	A	334	LYS
1	B	71	TRP
1	B	192	TYR
1	B	196	VAL
1	B	298	TYR
1	B	334	LYS
1	C	23	VAL
1	C	71	TRP
1	C	192	TYR
1	C	220	LEU
1	C	298	TYR
1	C	334	LYS
1	D	71	TRP
1	D	192	TYR
1	D	196	VAL
1	D	228	TYR
1	D	298	TYR
1	D	334	LYS
1	E	23	VAL
1	E	71	TRP
1	E	192	TYR
1	E	196	VAL
1	E	298	TYR
1	E	334	LYS
1	F	71	TRP

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Mol	Chain	Res	Type
1	F	192	TYR
1	F	196	VAL
1	F	197	ASN
1	F	220	LEU
1	F	298	TYR
1	F	334	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	167	HIS
1	A	210	HIS
1	A	275	ASN
1	A	278	ASN
1	A	281	HIS
1	B	20	GLN
1	B	138	ASN
1	B	167	HIS
1	B	197	ASN
1	B	210	HIS
1	B	281	HIS
1	B	292	HIS
1	C	20	GLN
1	C	138	ASN
1	C	167	HIS
1	C	210	HIS
1	C	249	ASN
1	C	275	ASN
1	C	278	ASN
1	D	138	ASN
1	D	167	HIS
1	D	197	ASN
1	D	210	HIS
1	D	249	ASN
1	D	275	ASN
1	D	278	ASN
1	D	281	HIS
1	D	292	HIS
1	E	138	ASN
1	E	167	HIS
1	E	197	ASN

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Mol	Chain	Res	Type
1	E	210	HIS
1	E	275	ASN
1	F	20	GLN
1	F	138	ASN
1	F	167	HIS
1	F	210	HIS
1	F	275	ASN

### 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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ARF	A	1335	-	2,2,2	2.12	1 (50%)	1,1,1	0.85	0
2	ARF	C	2335	-	2,2,2	2.13	1 (50%)	1,1,1	0.86	0
2	ARF	F	3335	-	2,2,2	2.19	1 (50%)	1,1,1	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARF	A	1335	-	-	0/0/0/0	0/0/0/0
2	ARF	C	2335	-	-	0/0/0/0	0/0/0/0
2	ARF	F	3335	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1335	ARF	O-C	2.94	1.33	1.22
2	C	2335	ARF	O-C	2.95	1.33	1.22
2	F	3335	ARF	O-C	3.04	1.33	1.22

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1335	ARF	2	0
2	C	2335	ARF	1	0

## 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, 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	317/334 (94%)	0.50	24 (7%) 17 24	24, 34, 42, 49	0
1	B	317/334 (94%)	0.56	37 (11%) 6 10	24, 35, 49, 52	0
1	C	317/334 (94%)	0.47	25 (7%) 15 22	25, 34, 44, 47	0
1	D	317/334 (94%)	0.51	25 (7%) 15 22	27, 36, 51, 56	0
1	E	316/334 (94%)	0.66	33 (10%) 8 12	28, 39, 55, 59	0
1	F	317/334 (94%)	0.74	38 (11%) 6 9	28, 39, 48, 51	0
All	All	1901/2004 (94%)	0.57	182 (9%) 10 15	24, 36, 48, 59	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	193	SER	12.6
1	A	229	TYR	11.8
1	F	228	TYR	11.7
1	F	229	TYR	11.0
1	B	192	TYR	10.8
1	A	228	TYR	10.6
1	B	228	TYR	10.1
1	B	229	TYR	8.5
1	D	229	TYR	8.5
1	C	229	TYR	8.4
1	E	192	TYR	8.2
1	E	229	TYR	7.9
1	C	228	TYR	7.7
1	B	193	SER	7.7
1	F	192	TYR	7.7
1	A	192	TYR	7.5
1	C	193	SER	7.4
1	C	222	GLY	7.3
1	E	228	TYR	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	192	TYR	6.7
1	D	228	TYR	6.7
1	F	24	PRO	6.6
1	F	193	SER	6.6
1	B	24	PRO	6.2
1	E	327	THR	6.2
1	D	192	TYR	6.1
1	C	25	ILE	5.8
1	D	24	PRO	5.8
1	A	193	SER	5.8
1	C	194	THR	5.6
1	A	24	PRO	5.4
1	F	191	GLY	5.4
1	E	191	GLY	5.2
1	C	230	PHE	5.2
1	F	194	THR	5.1
1	C	24	PRO	4.9
1	A	25	ILE	4.7
1	A	194	THR	4.6
1	B	191	GLY	4.6
1	A	230	PHE	4.6
1	D	25	ILE	4.5
1	D	193	SER	4.4
1	E	23	VAL	4.4
1	E	222	GLY	4.3
1	F	189	ILE	4.3
1	B	222	GLY	4.3
1	F	324	GLY	4.2
1	E	24	PRO	4.2
1	E	230	PHE	4.2
1	E	328	THR	4.1
1	B	25	ILE	4.1
1	D	334	LYS	4.1
1	D	328	THR	4.1
1	A	334	LYS	4.1
1	D	194	THR	4.1
1	A	231	GLY	4.0
1	D	222	GLY	3.9
1	D	333	GLY	3.9
1	D	230	PHE	3.8
1	C	23	VAL	3.8
1	B	23	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	314	HIS	3.7
1	A	222	GLY	3.6
1	B	333	GLY	3.6
1	F	23	VAL	3.6
1	D	323	TYR	3.6
1	F	41	ARG	3.5
1	C	191	GLY	3.5
1	B	194	THR	3.5
1	F	230	PHE	3.4
1	D	316	LYS	3.4
1	C	200	TRP	3.4
1	B	327	THR	3.4
1	D	191	GLY	3.4
1	D	321	SER	3.4
1	D	314	HIS	3.4
1	F	261	LYS	3.4
1	B	231	GLY	3.3
1	C	189	ILE	3.2
1	D	327	THR	3.2
1	A	189	ILE	3.2
1	E	333	GLY	3.2
1	B	230	PHE	3.2
1	A	163	VAL	3.2
1	B	328	THR	3.1
1	E	334	LYS	3.1
1	C	187	ILE	3.1
1	E	325	TYR	3.1
1	D	329	GLY	3.1
1	F	334	LYS	3.1
1	F	333	GLY	3.0
1	F	190	SER	2.9
1	F	231	GLY	2.9
1	F	164	CYS	2.9
1	A	325	TYR	2.9
1	A	190	SER	2.9
1	B	324	GLY	2.8
1	C	195	GLN	2.8
1	E	194	THR	2.7
1	B	195	GLN	2.7
1	A	23	VAL	2.7
1	B	165	ILE	2.7
1	F	25	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	306	LYS	2.6
1	F	188	ARG	2.6
1	C	165	ILE	2.6
1	D	322	ILE	2.6
1	E	111	ASN	2.6
1	C	163	VAL	2.6
1	E	319	ASP	2.5
1	E	306	LYS	2.5
1	E	322	ILE	2.5
1	C	172	PRO	2.5
1	B	171	ILE	2.5
1	B	322	ILE	2.5
1	B	334	LYS	2.5
1	E	261	LYS	2.5
1	F	165	ILE	2.5
1	A	197	ASN	2.5
1	F	195	GLN	2.5
1	B	320	GLY	2.5
1	D	326	PRO	2.5
1	D	304	ALA	2.5
1	F	197	ASN	2.5
1	E	304	ALA	2.4
1	F	169	GLY	2.4
1	F	293	ASP	2.4
1	F	314	HIS	2.4
1	E	195	GLN	2.4
1	F	280	GLY	2.4
1	B	93	LYS	2.4
1	B	189	ILE	2.4
1	C	306	LYS	2.4
1	E	231	GLY	2.4
1	E	273	GLU	2.4
1	F	316	LYS	2.4
1	A	165	ILE	2.4
1	B	163	VAL	2.4
1	E	200	TRP	2.4
1	C	334	LYS	2.4
1	C	169	GLY	2.3
1	E	272	LEU	2.3
1	B	323	TYR	2.3
1	C	231	GLY	2.3
1	F	166	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	332	PHE	2.3
1	B	295	GLY	2.3
1	F	232	GLU	2.3
1	D	23	VAL	2.3
1	E	171	ILE	2.3
1	E	330	GLY	2.3
1	F	313	ASP	2.3
1	E	27	ASN	2.3
1	A	164	CYS	2.2
1	A	232	GLU	2.2
1	E	113	ASN	2.2
1	B	218	VAL	2.2
1	D	100	VAL	2.2
1	A	288	PRO	2.2
1	F	222	GLY	2.2
1	B	196	VAL	2.2
1	D	41	ARG	2.2
1	F	111	ASN	2.2
1	C	166	SER	2.2
1	F	59	PRO	2.1
1	B	273	GLU	2.1
1	C	248	ARG	2.1
1	A	289	GLY	2.1
1	A	162	ALA	2.1
1	C	171	ILE	2.1
1	F	284	TYR	2.1
1	B	329	GLY	2.1
1	F	318	LYS	2.1
1	B	111	ASN	2.1
1	E	83	LYS	2.1
1	B	319	ASP	2.1
1	B	102	SER	2.1
1	B	57	ILE	2.1
1	B	200	TRP	2.0
1	A	248	ARG	2.0
1	F	163	VAL	2.0
1	F	321	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ARF	A	1335	3/3	0.83	0.27	0.33	36,36,40,40	0
2	ARF	C	2335	3/3	0.88	0.27	0.20	41,41,44,44	0
2	ARF	F	3335	3/3	0.90	0.28	-0.16	40,40,40,40	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.