



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:18 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

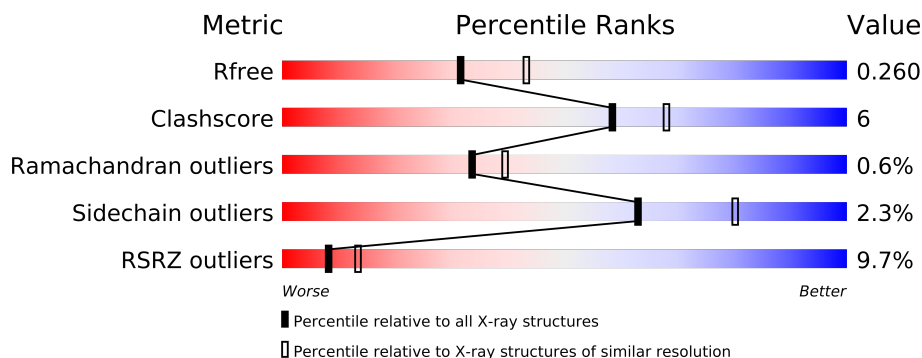
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance






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_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	334	
1	B	334	
1	C	334	
1	D	334	
1	E	334	
1	F	334	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15751 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

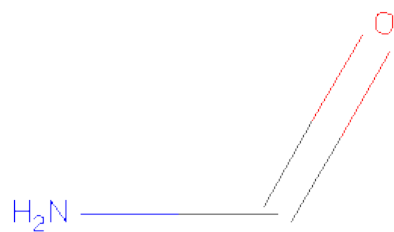
- Molecule 1 is a protein called Formamidase.

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: CH₃NO).



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		

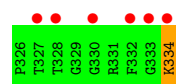
- Molecule 3 is water.

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		



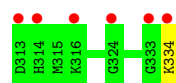
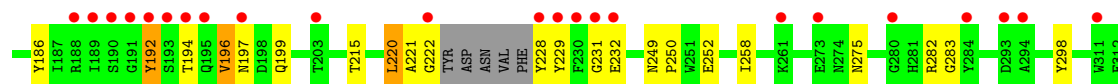
• Molecule 1: Formamidase

Chain E:



• Molecule 1: Formamidase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.253 , 0.285 0.253 , 0.260	Depositor DCC
R_{free} test set	4091 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.8	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	3	2	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (185) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:222:GLY:HA3	1:A:228:TYR:HB3	1.83	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

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%)	50	60
1	B	313/334 (94%)	298 (95%)	11 (4%)	4 (1%)	18	17
1	C	313/334 (94%)	298 (95%)	13 (4%)	2 (1%)	33	39
1	D	313/334 (94%)	302 (96%)	10 (3%)	1 (0%)	50	60
1	E	310/334 (93%)	299 (96%)	9 (3%)	2 (1%)	33	39
1	F	313/334 (94%)	299 (96%)	13 (4%)	1 (0%)	50	60
All	All	1875/2004 (94%)	1796 (96%)	68 (4%)	11 (1%)	33	39

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 ⓘ

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%)	63	80
1	B	263/277 (95%)	258 (98%)	5 (2%)	69	85
1	C	263/277 (95%)	257 (98%)	6 (2%)	63	80
1	D	263/277 (95%)	257 (98%)	6 (2%)	63	80
1	E	262/277 (95%)	256 (98%)	6 (2%)	63	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	263/277 (95%)	256 (97%)	7 (3%)	57	74
All	All	1577/1662 (95%)	1541 (98%)	36 (2%)	63	80

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
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
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 chains 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	1.96	1 (50%)	1,1,1	0.78	0
2	ARF	C	2335	-	2,2,2	1.96	1 (50%)	1,1,1	0.79	0
2	ARF	F	3335	-	2,2,2	2.02	1 (50%)	1,1,1	0.75	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	F	3335	ARF	O-C	2.74	1.33	1.23
2	C	2335	ARF	O-C	2.66	1.33	1.23
2	A	1335	ARF	O-C	2.65	1.33	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	317/334 (94%)	0.52	24 (7%)	14 20	24, 34, 42, 49	0
1	B	317/334 (94%)	0.58	35 (11%)	6 10	24, 35, 49, 52	0
1	C	317/334 (94%)	0.48	25 (7%)	13 19	25, 34, 44, 47	0
1	D	317/334 (94%)	0.55	26 (8%)	12 18	27, 36, 51, 56	0
1	E	316/334 (94%)	0.68	34 (10%)	6 10	28, 39, 55, 59	0
1	F	317/334 (94%)	0.76	40 (12%)	4 7	28, 39, 48, 51	0
All	All	1901/2004 (94%)	0.60	184 (9%)	8 13	24, 36, 48, 59	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	193	SER	12.3
1	A	229	TYR	11.7
1	F	228	TYR	11.2
1	B	192	TYR	10.8
1	A	228	TYR	10.7
1	B	228	TYR	10.5
1	F	229	TYR	10.3
1	E	192	TYR	8.8
1	D	229	TYR	8.6
1	B	229	TYR	8.2
1	C	228	TYR	8.1
1	B	193	SER	7.9
1	C	229	TYR	7.8
1	E	229	TYR	7.8
1	F	192	TYR	7.7
1	C	193	SER	7.7
1	E	228	TYR	7.3
1	A	192	TYR	7.3
1	C	222	GLY	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	192	TYR	7.2
1	F	24	PRO	7.0
1	D	228	TYR	6.8
1	F	193	SER	6.7
1	D	24	PRO	6.3
1	B	24	PRO	6.2
1	D	192	TYR	6.1
1	E	327	THR	6.1
1	C	25	ILE	5.9
1	C	194	THR	5.6
1	A	193	SER	5.4
1	A	24	PRO	5.4
1	F	191	GLY	5.3
1	E	191	GLY	5.1
1	C	24	PRO	5.0
1	F	194	THR	5.0
1	C	230	PHE	4.9
1	E	222	GLY	4.8
1	A	230	PHE	4.7
1	D	25	ILE	4.6
1	D	193	SER	4.4
1	E	24	PRO	4.4
1	B	191	GLY	4.4
1	A	25	ILE	4.4
1	B	25	ILE	4.4
1	B	222	GLY	4.3
1	D	328	THR	4.3
1	A	194	THR	4.3
1	E	23	VAL	4.1
1	D	222	GLY	4.1
1	E	230	PHE	3.9
1	C	23	VAL	3.9
1	D	194	THR	3.9
1	D	230	PHE	3.8
1	E	328	THR	3.8
1	D	333	GLY	3.8
1	F	189	ILE	3.8
1	D	323	TYR	3.8
1	A	334	LYS	3.7
1	F	23	VAL	3.7
1	D	327	THR	3.7
1	A	231	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	327	THR	3.7
1	B	23	VAL	3.6
1	E	314	HIS	3.6
1	F	324	GLY	3.6
1	A	222	GLY	3.6
1	B	194	THR	3.6
1	D	334	LYS	3.5
1	D	191	GLY	3.5
1	C	200	TRP	3.4
1	B	333	GLY	3.4
1	C	191	GLY	3.4
1	F	41	ARG	3.3
1	F	230	PHE	3.3
1	D	316	LYS	3.3
1	B	231	GLY	3.3
1	E	333	GLY	3.3
1	F	190	SER	3.2
1	E	322	ILE	3.2
1	D	314	HIS	3.1
1	E	325	TYR	3.1
1	F	261	LYS	3.1
1	C	187	ILE	3.1
1	B	230	PHE	3.1
1	D	329	GLY	3.1
1	F	231	GLY	3.1
1	D	322	ILE	3.0
1	B	328	THR	3.0
1	A	163	VAL	3.0
1	A	190	SER	2.9
1	F	333	GLY	2.9
1	C	189	ILE	2.9
1	F	164	CYS	2.9
1	F	25	ILE	2.8
1	A	189	ILE	2.8
1	E	304	ALA	2.8
1	D	321	SER	2.8
1	A	325	TYR	2.7
1	E	194	THR	2.7
1	B	165	ILE	2.7
1	C	172	PRO	2.7
1	D	326	PRO	2.7
1	A	23	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	195	GLN	2.7
1	C	165	ILE	2.7
1	E	334	LYS	2.6
1	E	111	ASN	2.6
1	C	195	GLN	2.6
1	B	322	ILE	2.6
1	E	306	LYS	2.5
1	F	334	LYS	2.5
1	F	165	ILE	2.5
1	F	293	ASP	2.5
1	E	231	GLY	2.5
1	C	163	VAL	2.5
1	A	232	GLU	2.5
1	F	280	GLY	2.5
1	B	93	LYS	2.5
1	A	197	ASN	2.5
1	B	324	GLY	2.4
1	F	232	GLU	2.4
1	B	306	LYS	2.4
1	C	231	GLY	2.4
1	F	169	GLY	2.4
1	E	261	LYS	2.4
1	B	171	ILE	2.4
1	E	27	ASN	2.4
1	B	329	GLY	2.4
1	C	169	GLY	2.4
1	F	188	ARG	2.4
1	F	314	HIS	2.4
1	F	316	LYS	2.4
1	B	320	GLY	2.4
1	A	165	ILE	2.4
1	C	166	SER	2.4
1	E	200	TRP	2.4
1	C	334	LYS	2.4
1	E	319	ASP	2.3
1	E	273	GLU	2.3
1	F	111	ASN	2.3
1	E	272	LEU	2.3
1	F	59	PRO	2.3
1	F	284	TYR	2.3
1	E	321	SER	2.3
1	D	23	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	332	PHE	2.2
1	E	195	GLN	2.2
1	B	163	VAL	2.2
1	F	166	SER	2.2
1	A	288	PRO	2.2
1	F	197	ASN	2.2
1	F	313	ASP	2.2
1	C	306	LYS	2.2
1	E	171	ILE	2.2
1	F	195	GLN	2.2
1	F	203	THR	2.2
1	D	304	ALA	2.2
1	A	164	CYS	2.2
1	E	113	ASN	2.2
1	B	189	ILE	2.1
1	C	248	ARG	2.1
1	D	41	ARG	2.1
1	A	162	ALA	2.1
1	B	102	SER	2.1
1	B	196	VAL	2.1
1	F	222	GLY	2.1
1	F	273	GLU	2.1
1	B	273	GLU	2.1
1	A	289	GLY	2.1
1	B	218	VAL	2.1
1	D	57	ILE	2.1
1	D	100	VAL	2.1
1	B	57	ILE	2.1
1	F	294	ALA	2.1
1	B	295	GLY	2.1
1	F	311	TRP	2.1
1	E	34	HIS	2.1
1	E	330	GLY	2.0
1	A	34	HIS	2.0
1	F	22	PRO	2.0
1	B	323	TYR	2.0
1	B	100	VAL	2.0
1	C	190	SER	2.0
1	B	200	TRP	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ARF	A	1335	3/3	0.27	0.40	36,36,40,40	0
2	ARF	C	2335	3/3	0.25	-0.05	41,41,44,44	0
2	ARF	F	3335	3/3	0.25	-0.40	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.