



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:12 PM UTC

PDB ID : 7W65 / pdb_00007w65
Title : Crystal structure of minor pilin TcpB from *Vibrio cholerae* complexed with secreted protein TcpF
Authors : Oki, H.; Kawahara, K.; Iimori, M.; Imoto, Y.; Maruno, T.; Uchiyama, S.; Muroga, Y.; Yoshida, A.; Yoshida, T.; Ohkubo, T.; Matsuda, S.; Iida, T.; Nakamura, S.
Deposited on : 2021-12-01
Resolution : 4.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

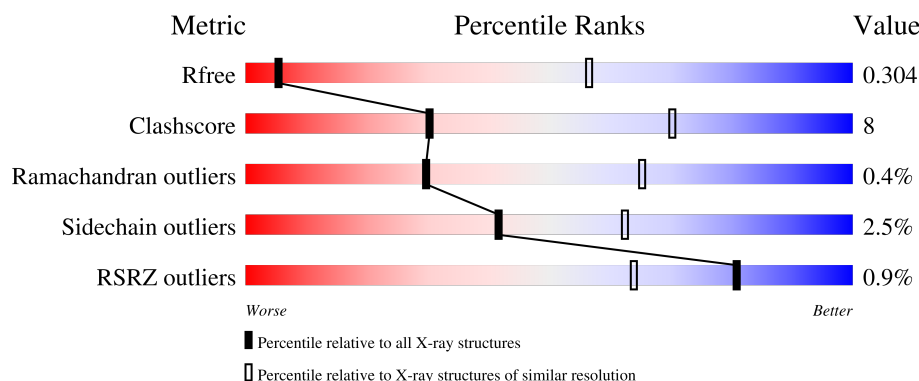
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.05 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}	180053	1183 (4.32-3.80)
Clashscore	190562	1231 (4.32-3.80)
Ramachandran outliers	187476	1154 (4.32-3.80)
Sidechain outliers	187428	1144 (4.32-3.80)
RSRZ outliers	180081	1182 (4.32-3.80)

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 ≥ 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	397	
1	B	397	
1	C	397	
2	D	318	
2	E	318	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	318	% 66% 28% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16441 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 Toxin-coregulated pilus biosynthesis protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3010	1883	511	608	8			
1	B	390	Total	C	N	O	S	0	0	0
			3010	1883	511	608	8			
1	C	395	Total	C	N	O	S	0	0	0
			3052	1911	517	615	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q9AGX1
A	28	GLY	-	expression tag	UNP Q9AGX1
B	27	GLY	-	expression tag	UNP Q9AGX1
B	28	GLY	-	expression tag	UNP Q9AGX1
C	27	GLY	-	expression tag	UNP Q9AGX1
C	28	GLY	-	expression tag	UNP Q9AGX1

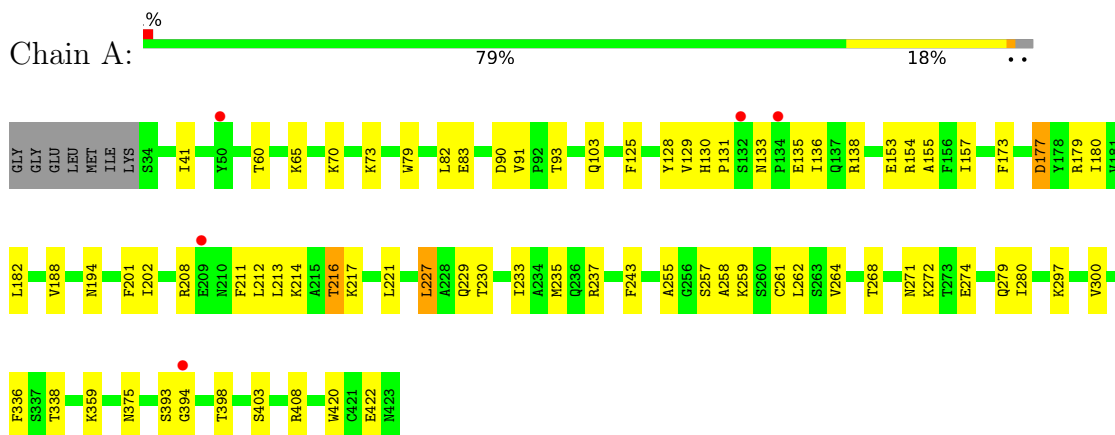
- Molecule 2 is a protein called Toxin coregulated pilus biosynthesis protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	307	Total	C	N	O	S	0	0	0
			2448	1561	397	482	8			
2	E	315	Total	C	N	O	S	0	0	0
			2506	1592	409	497	8			
2	F	302	Total	C	N	O	S	0	0	0
			2415	1543	392	472	8			

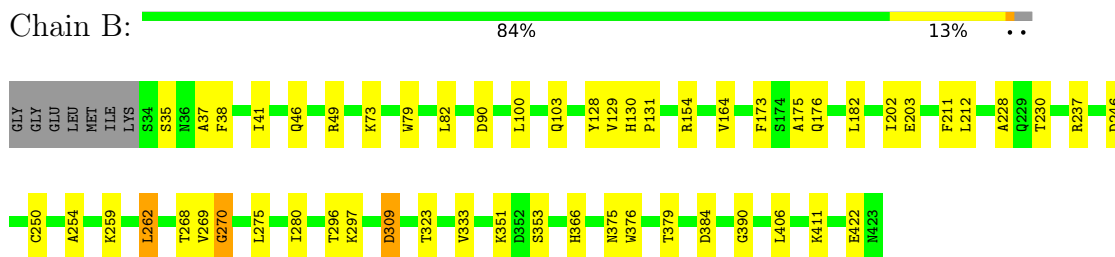
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

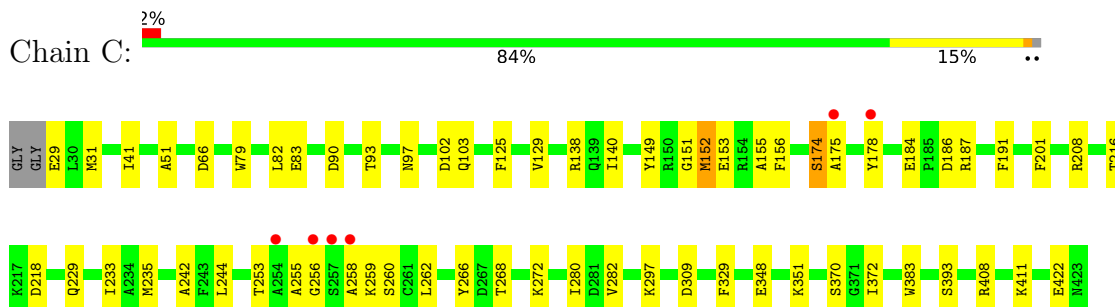
- Molecule 1: Toxin-coregulated pilus biosynthesis protein B



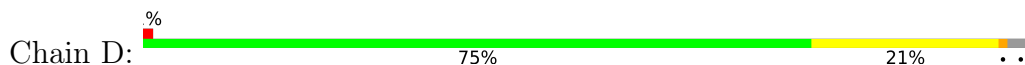
- Molecule 1: Toxin-coregulated pilus biosynthesis protein B

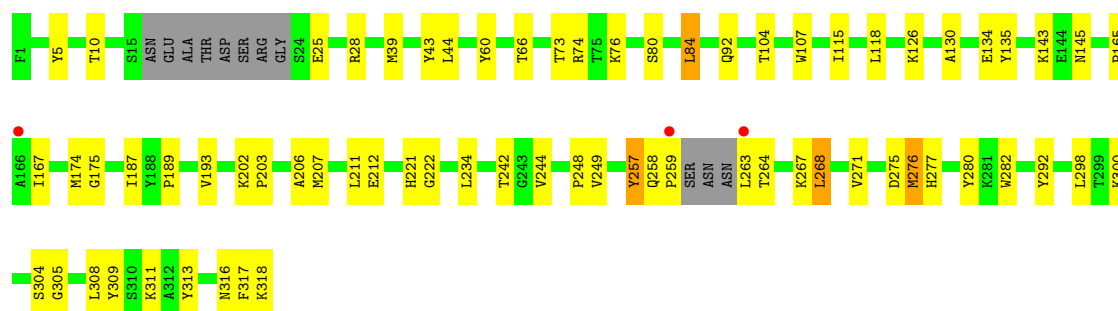


- Molecule 1: Toxin-coregulated pilus biosynthesis protein B

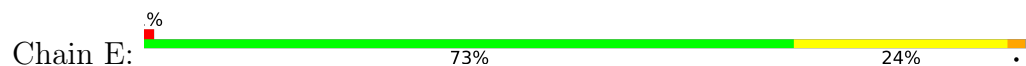


- Molecule 2: Toxin coregulated pilus biosynthesis protein F





- Molecule 2: Toxin coregulated pilus biosynthesis protein F



- Molecule 2: Toxin coregulated pilus biosynthesis protein F



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	284.14Å 284.14Å 297.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.83 – 4.05 31.83 – 4.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.83-4.05) 99.7 (31.83-4.05)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 4.00Å)	Xtriage
Refinement program	PHENIX v1.19.2-4092	Depositor
R, R_{free}	0.274 , 0.301 0.276 , 0.304	Depositor DCC
R_{free} test set	5718 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	185.5	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 199.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16441	wwPDB-VP
Average B, all atoms (Å ²)	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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	0.19	0/3065	0.45	0/4146
1	B	0.18	0/3065	0.41	0/4146
1	C	0.20	0/3107	0.45	0/4201
2	D	0.18	0/2505	0.46	0/3401
2	E	0.19	0/2564	0.43	1/3482 (0.0%)
2	F	0.18	0/2472	0.41	1/3356 (0.0%)
All	All	0.19	0/16778	0.43	2/22732 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	258	GLN	N-CA-C	5.97	119.34	110.32
2	E	264	THR	CB-CA-C	-5.44	108.54	116.53

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	3010	0	2920	55	0
1	B	3010	0	2920	43	0
1	C	3052	0	2970	45	0
2	D	2448	0	2378	45	0
2	E	2506	0	2428	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2415	0	2350	62	0
All	All	16441	0	15966	271	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 8.

All (271) 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:B:128:TYR:CZ	1:B:130:HIS:HA	2.09	0.88
1:B:128:TYR:OH	1:B:130:HIS:HA	1.75	0.87
1:A:131:PRO:HA	1:C:259:LYS:H	1.40	0.87
2:E:202:LYS:HE2	2:E:316:ASN:HD21	1.41	0.85
1:A:131:PRO:HB3	1:C:259:LYS:HB2	1.59	0.83
1:B:128:TYR:CE1	1:B:129:VAL:O	2.38	0.77
2:F:202:LYS:HE2	2:F:316:ASN:HD21	1.52	0.73
2:E:263:LEU:HB2	2:E:268:LEU:HD11	1.70	0.72
2:D:202:LYS:HE2	2:D:316:ASN:HD21	1.57	0.69
1:A:255:ALA:HB1	1:A:259:LYS:HE3	1.75	0.69
1:A:177:ASP:O	1:A:179:ARG:NH1	2.24	0.68
2:E:311:LYS:NZ	2:E:318:LYS:O	2.25	0.68
2:D:134:GLU:HG2	2:D:165:PRO:HB3	1.76	0.68
1:B:128:TYR:CD1	1:B:129:VAL:N	2.63	0.67
2:F:134:GLU:HG2	2:F:165:PRO:HB3	1.76	0.67
1:C:153:GLU:HB3	1:C:156:PHE:CD2	2.31	0.66
1:A:237:ARG:HA	1:C:235:MET:HE2	1.78	0.66
1:B:202:ILE:HG13	1:B:203:GLU:HG3	1.78	0.66
1:B:250:CYS:HB3	1:B:259:LYS:HG2	1.78	0.66
1:B:128:TYR:OH	1:B:131:PRO:HD3	1.96	0.65
2:F:207:MET:HB2	2:F:282:TRP:CH2	2.32	0.64
2:F:234:LEU:HD22	2:F:248:PRO:HG3	1.79	0.64
1:A:230:THR:HG22	1:B:100:LEU:HD13	1.79	0.64
2:F:263:LEU:HB2	2:F:268:LEU:HD11	1.79	0.63
1:C:309:ASP:HB3	1:C:411:LYS:HD2	1.81	0.63
2:D:298:LEU:HD23	2:D:308:LEU:HD12	1.81	0.62
2:E:38:GLY:HA3	2:E:129:THR:OG1	2.00	0.62
2:E:134:GLU:HG2	2:E:165:PRO:HB3	1.83	0.60
2:E:234:LEU:HD22	2:E:248:PRO:HG3	1.83	0.60
1:A:173:PHE:HD1	1:A:227:LEU:HD11	1.66	0.60
2:F:258:GLN:OE1	2:F:268:LEU:HB2	2.01	0.60
2:F:53:PRO:HB2	2:F:56:GLN:HG2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG21	1:C:253:THR:O	2.03	0.59
2:E:10:THR:O	2:E:16:ASN:ND2	2.35	0.59
1:A:173:PHE:CD1	1:A:227:LEU:HD11	2.38	0.59
2:D:258:GLN:OE1	2:D:268:LEU:HB2	2.02	0.59
2:E:218:LEU:HD13	2:E:226:LEU:HD22	1.85	0.59
1:A:257:SER:HA	1:B:131:PRO:HA	1.84	0.58
1:A:154:ARG:HH21	1:A:212:LEU:HB3	1.68	0.58
2:D:189:PRO:HD2	2:D:309:TYR:O	2.04	0.58
2:F:218:LEU:HD13	2:F:226:LEU:HD22	1.84	0.58
2:E:281:LYS:HA	2:E:284:ASN:HB2	1.86	0.57
2:E:242:THR:HG23	2:E:244:VAL:H	1.69	0.57
2:E:304:SER:OG	2:E:305:GLY:N	2.38	0.56
1:B:73:LYS:HB3	1:B:79:TRP:CD1	2.40	0.56
1:A:216:THR:OG1	1:A:217:LYS:N	2.38	0.56
2:E:201:LEU:HG	2:E:207:MET:HG3	1.88	0.56
2:E:258:GLN:HG3	2:E:270:ASN:HB3	1.87	0.56
2:F:115:ILE:HD13	2:F:118:LEU:HD12	1.87	0.56
1:B:297:LYS:NZ	1:B:422:GLU:OE1	2.39	0.56
1:B:154:ARG:HB3	1:B:212:LEU:HD22	1.88	0.56
1:C:79:TRP:HA	1:C:90:ASP:HB2	1.86	0.56
2:D:207:MET:HB2	2:D:282:TRP:CH2	2.41	0.56
2:F:263:LEU:N	2:F:267:LYS:HD3	2.21	0.55
2:F:189:PRO:HD2	2:F:309:TYR:O	2.07	0.55
2:D:107:TRP:HB3	2:D:167:ILE:HD12	1.89	0.55
2:E:187:ILE:HG21	2:E:221:HIS:CD2	2.42	0.55
1:B:376:TRP:HA	1:B:384:ASP:O	2.08	0.54
1:B:376:TRP:NE1	1:C:348:GLU:HB3	2.22	0.54
2:F:257:TYR:N	2:F:270:ASN:OD1	2.31	0.54
1:A:257:SER:O	1:A:259:LYS:N	2.37	0.54
2:F:281:LYS:HA	2:F:284:ASN:HB2	1.89	0.54
1:C:83:GLU:OE2	1:C:93:THR:OG1	2.24	0.54
2:D:257:TYR:CD1	2:D:257:TYR:C	2.85	0.54
2:D:275:ASP:OD2	2:D:282:TRP:HB3	2.08	0.54
2:E:23:GLY:HA3	2:E:61:ASP:HB3	1.91	0.53
1:C:408:ARG:NH2	2:F:3:ASP:OD1	2.30	0.53
1:B:46:GLN:OE1	1:B:49:ARG:NH1	2.41	0.53
2:F:258:GLN:HG3	2:F:270:ASN:HB3	1.90	0.53
1:C:216:THR:OG1	1:C:218:ASP:OD1	2.21	0.53
2:D:187:ILE:HG21	2:D:221:HIS:CD2	2.43	0.53
2:D:311:LYS:NZ	2:D:318:LYS:O	2.36	0.53
2:F:107:TRP:HB3	2:F:167:ILE:HD12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:258:GLN:OE1	2:E:268:LEU:HB2	2.09	0.53
2:F:66:THR:HG22	2:F:73:THR:HA	1.90	0.53
1:A:235:MET:HE2	1:A:243:PHE:CD1	2.44	0.52
1:B:254:ALA:HB3	1:C:266:TYR:CD1	2.44	0.52
2:D:10:THR:O	2:E:14:THR:OG1	2.22	0.52
2:F:201:LEU:HG	2:F:207:MET:HG3	1.92	0.52
1:A:153:GLU:HG3	1:A:155:ALA:H	1.75	0.52
1:C:153:GLU:HB3	1:C:156:PHE:HD2	1.75	0.52
2:E:193:VAL:HG22	2:E:211:LEU:HD22	1.90	0.52
2:F:52:PHE:CG	2:F:58:MET:HE3	2.45	0.52
2:F:202:LYS:HG2	2:F:203:PRO:HD2	1.91	0.52
1:A:157:ILE:HG23	1:A:180:ILE:HD13	1.92	0.52
1:B:82:LEU:HD11	1:B:103:GLN:HB3	1.92	0.52
2:D:234:LEU:HD22	2:D:248:PRO:HG3	1.90	0.52
2:E:275:ASP:OD2	2:E:282:TRP:HB3	2.10	0.52
1:A:131:PRO:HD3	1:C:259:LYS:NZ	2.24	0.52
2:E:205:GLY:HA2	2:E:280:TYR:CZ	2.44	0.52
2:F:242:THR:HG23	2:F:244:VAL:H	1.73	0.52
2:F:304:SER:OG	2:F:305:GLY:N	2.43	0.51
1:A:280:ILE:HG21	1:B:275:LEU:HB2	1.91	0.51
2:E:43:TYR:CE1	2:E:126:LYS:HE2	2.46	0.51
2:F:201:LEU:HB2	2:F:317:PHE:CE1	2.45	0.51
2:D:304:SER:OG	2:D:305:GLY:N	2.44	0.51
2:F:187:ILE:HG21	2:F:221:HIS:CD2	2.46	0.51
1:B:128:TYR:OH	1:B:131:PRO:CD	2.58	0.51
2:D:276:MET:HA	2:D:276:MET:HE2	1.92	0.51
1:C:393:SER:O	2:F:9:SER:HB2	2.11	0.51
2:E:189:PRO:HG3	2:E:308:LEU:HB3	1.93	0.51
1:C:329:PHE:HB2	1:C:383:TRP:CE2	2.46	0.50
2:D:249:VAL:HG21	2:D:292:TYR:OH	2.11	0.50
2:E:207:MET:HB2	2:E:282:TRP:CH2	2.47	0.50
1:B:73:LYS:HB3	1:B:79:TRP:NE1	2.25	0.50
1:B:353:SER:OG	1:B:366:HIS:NE2	2.36	0.50
2:E:20:ASP:OD1	2:E:21:SER:N	2.40	0.50
2:F:279:GLY:C	2:F:281:LYS:H	2.19	0.50
2:D:66:THR:HG22	2:D:74:ARG:H	1.76	0.50
1:A:237:ARG:NH1	1:C:242:ALA:O	2.43	0.50
2:E:70:GLY:HA2	2:F:12:TYR:CD1	2.47	0.50
2:E:189:PRO:HD2	2:E:309:TYR:O	2.12	0.50
1:A:157:ILE:HD13	1:A:180:ILE:HG23	1.94	0.50
1:C:175:ALA:HA	1:C:178:TYR:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:239:HIS:HB3	2:F:242:THR:HG22	1.93	0.49
2:F:298:LEU:HD23	2:F:308:LEU:HD12	1.92	0.49
1:B:128:TYR:CZ	1:B:130:HIS:CA	2.90	0.49
2:E:11:VAL:O	2:E:72:LYS:HD3	2.12	0.49
1:C:186:ASP:OD1	1:C:187:ARG:N	2.44	0.49
2:E:275:ASP:CG	2:E:282:TRP:HB3	2.37	0.49
2:F:276:MET:HG3	2:F:277:HIS:CE1	2.48	0.49
1:A:83:GLU:HG2	1:A:93:THR:HG23	1.94	0.49
1:B:128:TYR:CE1	1:B:129:VAL:C	2.90	0.49
1:C:174:SER:OG	1:C:175:ALA:N	2.45	0.49
2:E:139:ARG:HD3	2:E:160:THR:O	2.13	0.49
1:A:237:ARG:HG2	1:C:244:LEU:HG	1.94	0.49
2:F:313:TYR:HB3	2:F:317:PHE:HA	1.94	0.49
1:A:182:LEU:HG	1:A:211:PHE:CZ	2.48	0.49
1:B:128:TYR:OH	1:B:130:HIS:CD2	2.66	0.49
1:B:309:ASP:HA	1:B:411:LYS:HD2	1.95	0.48
2:F:250:TYR:OH	2:F:252:GLU:OE1	2.24	0.48
1:A:130:HIS:CG	1:A:131:PRO:HD2	2.48	0.48
2:E:213:TYR:O	2:E:266:LYS:HB3	2.13	0.48
1:A:154:ARG:HB2	1:A:154:ARG:CZ	2.43	0.48
2:F:60:TYR:CZ	2:F:76:LYS:HA	2.48	0.48
1:C:29:GLU:HG3	1:C:31:MET:HG3	1.95	0.48
1:C:260:SER:HB2	1:C:280:ILE:HG12	1.95	0.48
2:F:139:ARG:CZ	2:F:150:ILE:HG21	2.43	0.48
1:B:176:GLN:HG2	1:B:228:ALA:HB3	1.94	0.48
1:A:375:ASN:OD1	1:B:351:LYS:HG2	2.12	0.48
1:B:406:LEU:HD21	2:D:5:TYR:HB3	1.96	0.48
2:E:22:ARG:HG2	2:E:61:ASP:HA	1.96	0.48
1:A:233:ILE:HD12	1:B:237:ARG:CZ	2.44	0.48
1:C:153:GLU:HG3	1:C:155:ALA:H	1.79	0.48
1:A:129:VAL:HG22	1:C:256:GLY:O	2.13	0.47
1:A:338:THR:HG23	1:C:370:SER:O	2.14	0.47
2:E:107:TRP:HB3	2:E:167:ILE:HD12	1.96	0.47
1:C:184:GLU:HG3	1:C:191:PHE:CE1	2.50	0.47
1:C:82:LEU:HD11	1:C:103:GLN:HB3	1.97	0.47
2:E:202:LYS:HG2	2:E:203:PRO:HD2	1.95	0.47
2:F:234:LEU:HB3	2:F:248:PRO:HB3	1.96	0.47
1:B:375:ASN:OD1	1:C:351:LYS:HG2	2.13	0.47
1:C:51:ALA:O	1:C:140:ILE:HD12	2.14	0.47
2:D:313:TYR:HB3	2:D:317:PHE:HA	1.96	0.47
1:B:250:CYS:SG	1:B:259:LYS:HE3	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:THR:HG23	1:C:255:ALA:H	1.79	0.47
2:D:115:ILE:HD13	2:D:118:LEU:HD12	1.96	0.47
2:D:212:GLU:HA	2:D:268:LEU:HA	1.97	0.47
2:D:206:ALA:HA	2:D:275:ASP:CG	2.39	0.47
1:A:271:ASN:O	1:A:272:LYS:HD2	2.15	0.47
1:B:173:PHE:CE2	1:B:175:ALA:HB2	2.50	0.47
2:D:28:ARG:NH1	2:E:17:GLU:OE1	2.40	0.47
2:F:311:LYS:NZ	2:F:318:LYS:O	2.44	0.47
1:C:297:LYS:NZ	1:C:422:GLU:OE1	2.47	0.46
2:F:242:THR:HG21	2:F:246:TYR:OH	2.15	0.46
2:D:222:GLY:O	2:D:300:LYS:NZ	2.42	0.46
2:F:193:VAL:HG22	2:F:211:LEU:HD22	1.96	0.46
2:D:263:LEU:N	2:D:267:LYS:HD3	2.31	0.46
2:F:231:PHE:CD2	2:F:256:PRO:HG3	2.51	0.46
1:A:300:VAL:HG12	1:A:420:TRP:HB3	1.97	0.46
2:E:267:LYS:HD3	2:E:267:LYS:HA	1.79	0.46
2:F:285:THR:O	2:F:292:TYR:HD2	1.99	0.46
1:A:70:LYS:O	1:A:188:VAL:HG11	2.16	0.46
1:A:73:LYS:HB3	1:A:79:TRP:CE2	2.51	0.46
1:B:182:LEU:HG	1:B:211:PHE:CZ	2.51	0.46
2:D:66:THR:HG22	2:D:73:THR:HA	1.97	0.45
2:D:130:ALA:O	2:D:134:GLU:HB2	2.15	0.45
1:C:66:ASP:HB3	1:C:138:ARG:CZ	2.47	0.45
2:E:205:GLY:HA2	2:E:280:TYR:CE1	2.51	0.45
2:F:66:THR:HG22	2:F:74:ARG:H	1.81	0.45
2:D:43:TYR:CE1	2:D:126:LYS:HE2	2.52	0.45
2:D:174:MET:HE3	2:D:175:GLY:H	1.80	0.45
2:F:118:LEU:HD13	2:F:135:TYR:CZ	2.52	0.45
2:E:191:ILE:HD12	2:E:211:LEU:HD13	1.98	0.45
2:E:17:GLU:OE2	2:E:72:LYS:NZ	2.45	0.45
1:B:35:SER:HA	1:B:38:PHE:HB3	1.98	0.45
1:C:149:TYR:CZ	1:C:151:GLY:HA3	2.52	0.45
2:D:257:TYR:O	2:D:257:TYR:CG	2.69	0.45
2:F:264:THR:C	2:F:266:LYS:H	2.25	0.45
2:D:276:MET:HE3	2:D:280:TYR:CE2	2.51	0.44
2:F:223:TYR:CE1	2:F:300:LYS:HE3	2.52	0.44
2:D:259:PRO:O	2:D:263:LEU:HD13	2.17	0.44
2:E:257:TYR:N	2:E:270:ASN:OD1	2.39	0.44
2:F:64:PRO:HD2	2:F:74:ARG:NH2	2.31	0.44
1:B:230:THR:HB	1:C:102:ASP:OD1	2.16	0.44
2:D:202:LYS:HG2	2:D:203:PRO:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:LYS:HA	2:F:147:ARG:O	2.18	0.44
1:A:257:SER:C	1:A:259:LYS:H	2.25	0.44
2:F:231:PHE:HD2	2:F:256:PRO:HG3	1.83	0.44
2:F:258:GLN:HB2	2:F:269:TYR:HA	2.00	0.44
2:F:275:ASP:HB3	2:F:280:TYR:HA	1.99	0.44
1:A:264:VAL:HG11	1:C:260:SER:OG	2.17	0.44
2:F:39:MET:SD	2:F:44:LEU:HD12	2.57	0.44
1:A:73:LYS:HA	1:A:73:LYS:HD2	1.87	0.43
2:E:209:ALA:HB2	2:E:317:PHE:HZ	1.82	0.43
1:A:173:PHE:HB3	1:A:227:LEU:HD21	1.98	0.43
1:A:182:LEU:HD23	1:A:221:LEU:HA	2.01	0.43
1:A:128:TYR:CG	1:A:129:VAL:N	2.86	0.43
1:A:201:PHE:HD2	1:A:202:ILE:HD12	1.83	0.43
1:A:359:LYS:HB3	1:A:359:LYS:HE2	1.68	0.43
1:A:403:SER:OG	1:A:408:ARG:NH1	2.52	0.43
1:B:79:TRP:HA	1:B:90:ASP:HB2	2.00	0.43
1:B:268:THR:C	1:B:270:GLY:H	2.27	0.43
2:D:118:LEU:HD13	2:D:135:TYR:CZ	2.53	0.43
1:C:272:LYS:HA	1:C:272:LYS:HD3	1.84	0.43
2:F:226:LEU:HB3	2:F:269:TYR:OH	2.19	0.43
1:A:82:LEU:HD11	1:A:103:GLN:HB3	2.01	0.43
2:E:37:ILE:HD13	2:E:58:MET:HE1	2.01	0.43
1:B:296:THR:O	1:B:422:GLU:HA	2.19	0.43
2:E:174:MET:HE3	2:E:175:GLY:H	1.84	0.43
1:C:309:ASP:CB	1:C:411:LYS:HD2	2.48	0.43
2:E:233:VAL:HG12	2:E:252:GLU:HB3	2.00	0.43
2:D:25:GLU:OE2	2:F:26:HIS:HA	2.19	0.42
1:A:41:ILE:HD13	1:A:41:ILE:HA	1.80	0.42
1:B:37:ALA:HB1	1:B:164:VAL:HA	2.02	0.42
1:B:128:TYR:CG	1:B:129:VAL:N	2.87	0.42
1:C:152:MET:HB2	1:C:152:MET:HE3	1.62	0.42
1:C:201:PHE:O	1:C:208:ARG:HD3	2.19	0.42
1:C:229:GLN:HB3	1:C:233:ILE:HG13	2.01	0.42
2:F:82:ARG:HD3	2:F:90:SER:OG	2.19	0.42
2:F:174:MET:HE3	2:F:175:GLY:H	1.84	0.42
1:A:297:LYS:NZ	1:A:422:GLU:OE1	2.51	0.42
2:D:193:VAL:HG22	2:D:211:LEU:HD22	2.02	0.42
1:A:60:THR:HG23	1:A:136:ILE:HD11	2.01	0.42
1:A:125:PHE:CG	1:A:138:ARG:HD2	2.55	0.42
1:A:336:PHE:CE1	1:C:372:ILE:HB	2.54	0.42
2:D:60:TYR:CZ	2:D:76:LYS:HA	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:82:ARG:HB2	2:E:91:LEU:HD21	2.01	0.42
2:F:145:ASN:OD1	2:F:145:ASN:N	2.52	0.42
2:E:247:ASP:OD1	2:E:247:ASP:N	2.53	0.42
2:F:231:PHE:CZ	2:F:298:LEU:HD13	2.55	0.42
2:D:92:GLN:OE1	2:D:143:LYS:NZ	2.51	0.42
2:D:263:LEU:HD12	2:D:263:LEU:HA	1.72	0.41
2:F:215:VAL:HG23	2:F:266:LYS:HA	2.02	0.41
1:A:214:LYS:O	1:A:216:THR:HG22	2.19	0.41
2:E:257:TYR:O	2:E:257:TYR:CG	2.70	0.41
2:F:203:PRO:HD3	2:F:287:PHE:CZ	2.55	0.41
1:A:65:LYS:HA	1:A:135:GLU:O	2.21	0.41
1:C:125:PHE:CG	1:C:138:ARG:HD2	2.56	0.41
2:D:242:THR:HG23	2:D:244:VAL:H	1.85	0.41
2:D:39:MET:SD	2:D:44:LEU:HD12	2.61	0.41
2:D:104:THR:HB	2:D:107:TRP:CZ2	2.55	0.41
2:E:60:TYR:CZ	2:E:76:LYS:HA	2.55	0.41
1:A:82:LEU:HA	1:A:91:VAL:HB	2.03	0.41
1:B:262:LEU:HD23	1:B:280:ILE:HD11	2.02	0.41
2:D:80:SER:O	2:D:84:LEU:HD22	2.20	0.41
1:A:261:CYS:HB2	1:A:279:GLN:OE1	2.21	0.41
1:A:79:TRP:HA	1:A:90:ASP:HB2	2.02	0.41
1:A:274:GLU:HA	1:C:282:VAL:HG23	2.03	0.41
2:E:220:LYS:HA	2:E:220:LYS:HD2	1.95	0.41
1:B:41:ILE:HD13	1:B:41:ILE:HA	1.81	0.41
1:B:390:GLY:HA3	2:D:5:TYR:CE1	2.56	0.41
2:D:280:TYR:O	2:D:282:TRP:N	2.54	0.41
2:F:187:ILE:HG21	2:F:221:HIS:HD2	1.84	0.41
2:F:141:LEU:HD23	2:F:164:LEU:HD22	2.02	0.40
2:F:257:TYR:O	2:F:257:TYR:CG	2.70	0.40
1:A:394:GLY:HA3	2:E:12:TYR:CE2	2.57	0.40
1:C:41:ILE:HD13	1:C:41:ILE:HA	1.88	0.40
2:E:258:GLN:HB2	2:E:269:TYR:HA	2.02	0.40
2:F:66:THR:HG21	2:F:75:THR:HG23	2.03	0.40
2:E:92:GLN:HA	2:E:96:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/397 (98%)	371 (96%)	15 (4%)	2 (0%)	24	61
1	B	388/397 (98%)	374 (96%)	12 (3%)	2 (0%)	24	61
1	C	393/397 (99%)	378 (96%)	13 (3%)	2 (0%)	24	61
2	D	301/318 (95%)	279 (93%)	21 (7%)	1 (0%)	36	70
2	E	311/318 (98%)	292 (94%)	18 (6%)	1 (0%)	36	70
2	F	296/318 (93%)	277 (94%)	18 (6%)	1 (0%)	36	70
All	All	2077/2145 (97%)	1971 (95%)	97 (5%)	9 (0%)	30	65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	271	VAL
2	E	271	VAL
1	A	258	ALA
1	C	174	SER
2	F	271	VAL
1	B	270	GLY
1	C	258	ALA
1	A	177	ASP
1	B	269	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	329/334 (98%)	318 (97%)	11 (3%)	33	56
1	B	329/334 (98%)	323 (98%)	6 (2%)	51	68
1	C	334/334 (100%)	329 (98%)	5 (2%)	57	71
2	D	272/281 (97%)	265 (97%)	7 (3%)	40	61
2	E	278/281 (99%)	267 (96%)	11 (4%)	28	50
2	F	268/281 (95%)	263 (98%)	5 (2%)	50	67
All	All	1810/1845 (98%)	1765 (98%)	45 (2%)	42	62

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	194	ASN
1	A	208	ARG
1	A	213	LEU
1	A	216	THR
1	A	227	LEU
1	A	229	GLN
1	A	262	LEU
1	A	268	THR
1	A	393	SER
1	A	398	THR
1	B	246	ASP
1	B	262	LEU
1	B	309	ASP
1	B	323	THR
1	B	333	VAL
1	B	379	THR
1	C	97	ASN
1	C	129	VAL
1	C	152	MET
1	C	262	LEU
1	C	268	THR
2	D	84	LEU
2	D	145	ASN
2	D	257	TYR
2	D	264	THR
2	D	268	LEU
2	D	276	MET
2	D	277	HIS
2	E	11	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	14	THR
2	E	15	SER
2	E	16	ASN
2	E	17	GLU
2	E	84	LEU
2	E	145	ASN
2	E	264	THR
2	E	268	LEU
2	E	277	HIS
2	E	280	TYR
2	F	11	VAL
2	F	12	TYR
2	F	84	LEU
2	F	145	ASN
2	F	268	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	194	ASN
1	B	122	GLN
1	B	236	GLN
1	B	341	GLN
1	C	97	ASN
1	C	101	GLN
1	C	103	GLN
1	C	229	GLN
2	D	123	ASN
2	D	316	ASN
2	E	123	ASN
2	E	316	ASN
2	F	123	ASN
2	F	185	ASN
2	F	316	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	390/397 (98%)	-0.21	5 (1%) 75 57	155, 239, 282, 297	0
1	B	390/397 (98%)	-0.29	0 100 100	157, 197, 226, 267	0
1	C	395/397 (99%)	-0.24	6 (1%) 72 54	155, 209, 241, 273	0
2	D	307/318 (96%)	-0.22	3 (0%) 79 61	192, 235, 298, 308	0
2	E	315/318 (99%)	-0.35	3 (0%) 79 61	185, 234, 340, 348	0
2	F	302/318 (94%)	-0.32	2 (0%) 84 69	204, 228, 279, 295	0
All	All	2099/2145 (97%)	-0.27	19 (0%) 81 64	155, 218, 308, 348	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	256	GLY	5.9
2	F	259	PRO	4.7
1	C	257	SER	4.1
2	D	259	PRO	3.6
2	F	263	LEU	3.6
1	A	134	PRO	3.3
1	C	258	ALA	3.3
1	C	254	ALA	2.9
1	A	132	SER	2.9
1	C	175	ALA	2.7
1	A	209	GLU	2.7
2	E	259	PRO	2.7
1	A	50	TYR	2.6
2	E	263	LEU	2.5
2	D	263	LEU	2.5
1	C	178	TYR	2.4
2	D	166	ALA	2.3
1	A	394	GLY	2.2
2	E	12	TYR	2.1

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 oligosaccharides 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.