Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 12:41 PM JST

PDB ID	:	7W65
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:

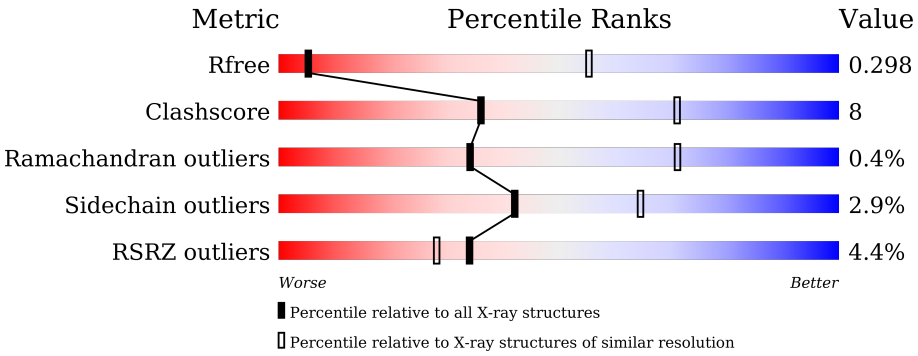
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1127 (4.42-3.70)
Clashscore	141614	1033 (4.40-3.72)
Ramachandran outliers	138981	1145 (4.42-3.70)
Sidechain outliers	138945	1133 (4.42-3.70)
RSRZ outliers	127900	1005 (4.44-3.68)

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 <=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	5% 80% 17%
1	B	397	% 85% 13%
1	C	397	% 84% 15%
2	D	318	6% 75% 20%
2	E	318	9% 74% 22%
2	F	318	7% 68% 25% 5%

2 Entry composition (i)

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.

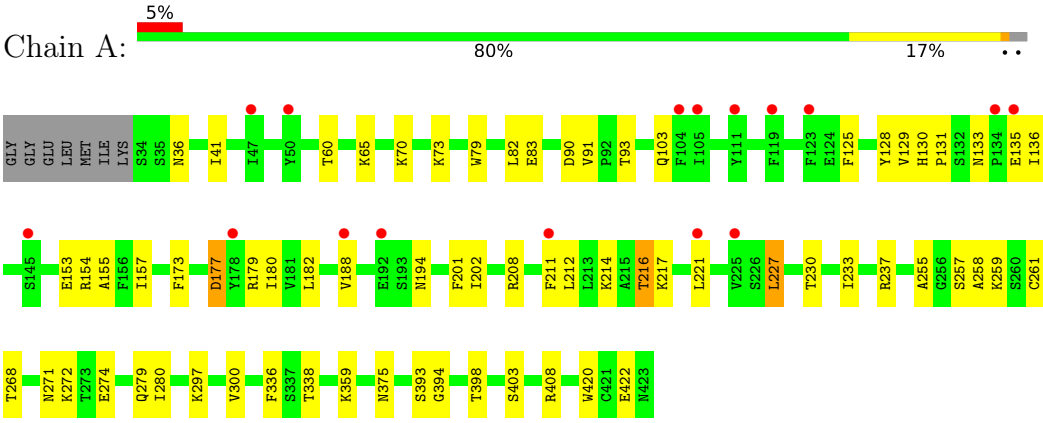
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	307	Total	C	N	O	S	0	0	0
			2448	1561	397	482	8			
2	E	315	Total	C	N	O	S	0	0	0
			2506	1592	409	497	8			
2	F	302	Total	C	N	O	S	0	0	0
			2415	1543	392	472	8			

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.

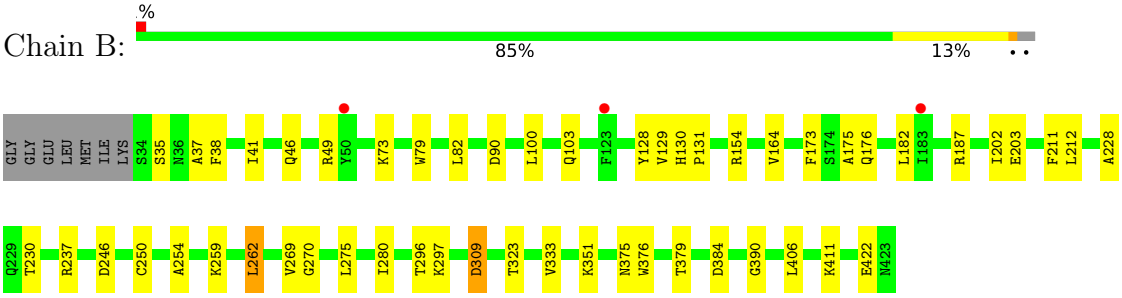
• Molecule 1: Toxin-coregulated pilus biosynthesis protein B

Chain A:



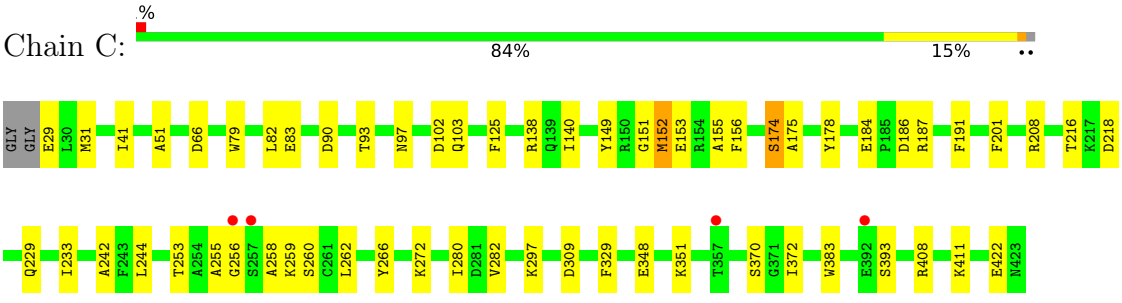
• Molecule 1: Toxin-coregulated pilus biosynthesis protein B

Chain B:



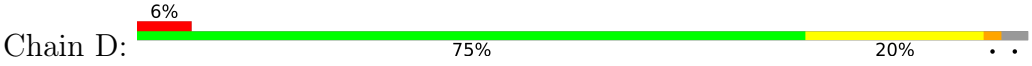
• Molecule 1: Toxin-coregulated pilus biosynthesis protein B

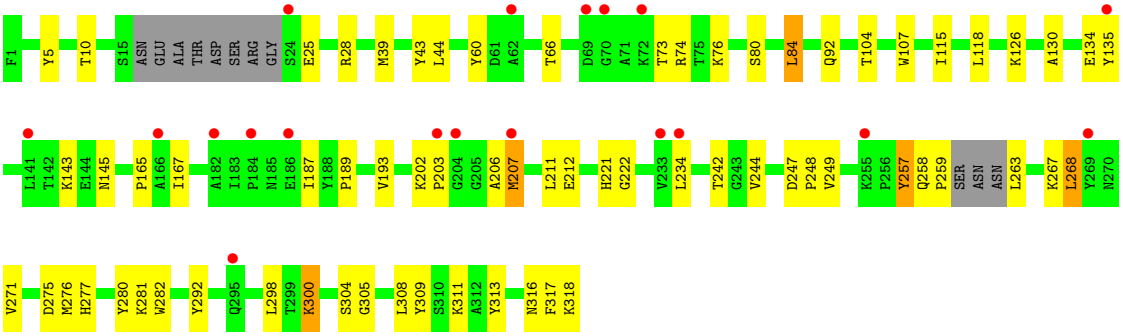
Chain C:



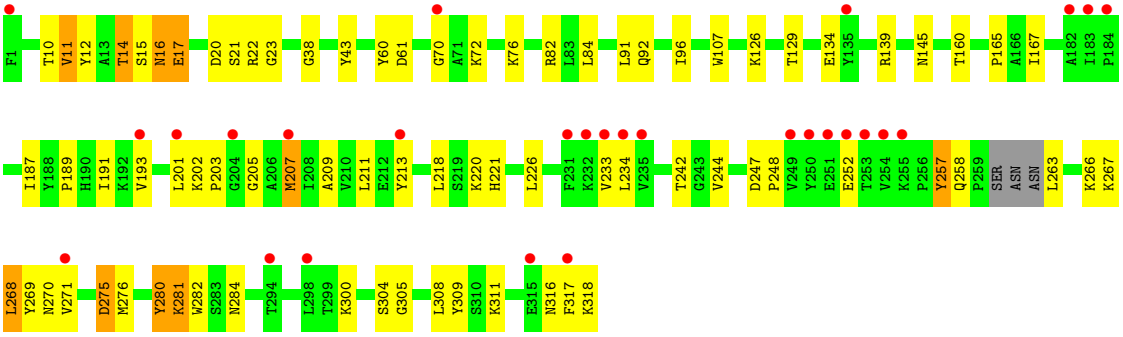
• Molecule 2: Toxin coregulated pilus biosynthesis protein F

Chain D:

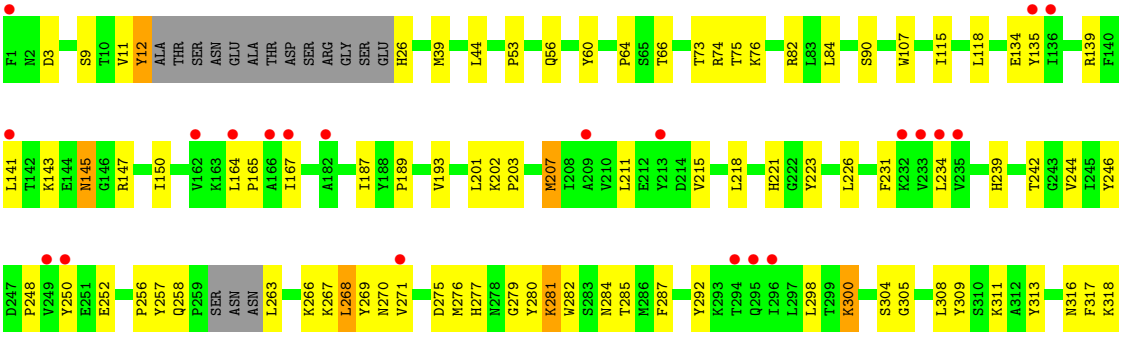




• Molecule 2: Toxin coregulated pilus biosynthesis protein F



• Molecule 2: Toxin coregulated pilus biosynthesis protein F



4 Data and refinement statistics (i)

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 49.21 – 4.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.83-4.05) 99.9 (49.21-4.05)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 4.00Å)	Xtriage
Refinement program	PHENIX v1.19.2-4092	Depositor
R, R_{free}	0.274 , 0.301 0.273 , 0.298	Depositor DCC
R_{free} test set	5716 reflections (9.87%)	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 , 188.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.29	0/3065	0.51	0/4146
1	B	0.29	0/3065	0.50	0/4146
1	C	0.30	0/3107	0.52	0/4201
2	D	0.28	0/2505	0.51	0/3401
2	E	0.28	0/2564	0.49	0/3482
2	F	0.28	0/2472	0.48	0/3356
All	All	0.29	0/16778	0.50	0/22732

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

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	52	0
1	B	3010	0	2920	41	0
1	C	3052	0	2970	44	0
2	D	2448	0	2378	43	0
2	E	2506	0	2428	50	0
2	F	2415	0	2350	59	0
All	All	16441	0	15966	260	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 (260) 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: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
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:D:311:LYS:NZ	2:D:318:LYS:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:GLY:HA3	2:E:129:THR:HG1	1.70	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: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
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:F:107:TRP:HB3	2:F:167:ILE:HD12	1.90	0.53
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:20:ASP:OD1	2:E:21:SER:N	2.40	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
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
2:F:250:TYR:OH	2:F:252:GLU:OE1	2.24	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: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:297:LYS:NZ	1:B:422:GLU:OE1	2.39	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
2:D:257:TYR:CD1	2:D:257:TYR:C	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:HA	1:B:411:LYS:HD2	1.95	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:257:TYR:O	2:D:257:TYR:CG	2.69	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: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:F:279:GLY:C	2:F:281:LYS:H	2.19	0.45
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:E:275:ASP:CG	2:E:282:TRP:HB3	2.37	0.44
2:F:64:PRO:HD2	2:F:74:ARG:NH2	2.31	0.44
1:B:128:TYR:CE1	1:B:129:VAL:C	2.90	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
2:F:143:LYS:HA	2:F:147:ARG:O	2.18	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:C:152:MET:HE3	1:C:152:MET:HB2	1.78	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
2:D:118:LEU:HD13	2:D:135:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:296:THR:O	1:B:422:GLU:HA	2.19	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: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
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
2:D:206:ALA:HA	2:D:275:ASP:CG	2.39	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
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
1:C:83:GLU:OE2	1:C:93:THR:OG1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:247:ASP:N	2:D:247:ASP:OD1	2.54	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%)	29	67
1	B	388/397 (98%)	374 (96%)	12 (3%)	2 (0%)	29	67
1	C	393/397 (99%)	378 (96%)	13 (3%)	2 (0%)	29	67
2	D	301/318 (95%)	279 (93%)	21 (7%)	1 (0%)	41	75
2	E	311/318 (98%)	292 (94%)	18 (6%)	1 (0%)	41	75
2	F	296/318 (93%)	277 (94%)	18 (6%)	1 (0%)	41	75
All	All	2077/2145 (97%)	1971 (95%)	97 (5%)	9 (0%)	34	71

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%)	319 (97%)	10 (3%)	41	64
1	B	329/334 (98%)	322 (98%)	7 (2%)	53	72
1	C	334/334 (100%)	331 (99%)	3 (1%)	78	88
2	D	272/281 (97%)	263 (97%)	9 (3%)	38	62
2	E	278/281 (99%)	263 (95%)	15 (5%)	22	50
2	F	268/281 (95%)	260 (97%)	8 (3%)	41	64
All	All	1810/1845 (98%)	1758 (97%)	52 (3%)	42	64

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	133	ASN
1	A	194	ASN
1	A	208	ARG
1	A	216	THR
1	A	227	LEU
1	A	262	LEU
1	A	268	THR
1	A	393	SER
1	A	398	THR

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Mol	Chain	Res	Type
1	B	187	ARG
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	152	MET
1	C	262	LEU
2	D	84	LEU
2	D	145	ASN
2	D	207	MET
2	D	257	TYR
2	D	268	LEU
2	D	276	MET
2	D	277	HIS
2	D	281	LYS
2	D	300	LYS
2	E	11	VAL
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	207	MET
2	E	257	TYR
2	E	268	LEU
2	E	275	ASP
2	E	276	MET
2	E	280	TYR
2	E	281	LYS
2	E	300	LYS
2	F	11	VAL
2	F	12	TYR
2	F	84	LEU
2	F	145	ASN
2	F	207	MET
2	F	268	LEU
2	F	281	LYS
2	F	300	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	316	ASN
2	E	316	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

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^{th} 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	18 (4%) 32 27	155, 239, 282, 297	0
1	B	390/397 (98%)	0.02	3 (0%) 86 79	157, 197, 226, 267	0
1	C	395/397 (99%)	0.07	4 (1%) 82 74	155, 209, 241, 273	0
2	D	307/318 (96%)	0.28	19 (6%) 20 17	192, 235, 298, 308	0
2	E	315/318 (99%)	0.38	28 (8%) 9 8	185, 234, 340, 348	0
2	F	302/318 (94%)	0.24	21 (6%) 16 13	204, 228, 279, 295	0
All	All	2099/2145 (97%)	0.19	93 (4%) 34 28	155, 218, 308, 348	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	SER	8.5
2	E	294	THR	4.5
2	F	234	LEU	4.1
2	E	135	TYR	3.9
1	A	134	PRO	3.9
2	E	250	TYR	3.9
1	A	50	TYR	3.9
2	F	135	TYR	3.8
2	D	72	LYS	3.7
2	F	233	VAL	3.7
2	F	249	VAL	3.6
1	A	135	GLU	3.6
1	A	119	PHE	3.5
1	C	256	GLY	3.5
2	E	233	VAL	3.5
2	F	1	PHE	3.5
2	E	252	GLU	3.4
2	F	166	ALA	3.4
2	F	136	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	141	LEU	3.3
2	E	254	VAL	3.3
2	D	166	ALA	3.3
2	F	232	LYS	3.2
1	C	357	THR	3.2
2	D	186	GLU	3.1
2	D	233	VAL	3.1
2	D	182	ALA	3.1
1	A	105	ILE	3.1
2	D	234	LEU	3.0
2	F	209	ALA	3.0
2	E	204	GLY	2.9
2	E	232	LYS	2.9
2	F	182	ALA	2.8
2	E	213	TYR	2.7
1	A	225	VAL	2.7
2	D	269	TYR	2.7
2	F	235	VAL	2.7
2	E	182	ALA	2.7
2	E	235	VAL	2.6
2	F	294	THR	2.6
2	E	249	VAL	2.6
2	E	234	LEU	2.6
2	D	135	TYR	2.6
2	F	167	ILE	2.6
1	A	178	TYR	2.6
2	E	231	PHE	2.6
2	E	253	THR	2.5
2	E	184	PRO	2.5
2	F	250	TYR	2.5
1	A	111	TYR	2.5
2	F	164	LEU	2.5
1	B	50	TYR	2.4
2	F	141	LEU	2.4
2	F	296	ILE	2.4
1	A	192	GLU	2.4
2	D	69	ASP	2.4
2	E	70	GLY	2.4
2	E	207	MET	2.4
2	D	24	SER	2.3
2	F	213	TYR	2.3
1	A	104	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	145	SER	2.3
2	D	70	GLY	2.3
1	B	183	ILE	2.3
1	A	47	ILE	2.3
2	D	255	LYS	2.3
2	E	193	VAL	2.2
2	E	255	LYS	2.2
2	D	184	PRO	2.2
2	E	315	GLU	2.2
1	A	123	PHE	2.2
1	A	221	LEU	2.2
2	E	201	LEU	2.2
1	A	140	ILE	2.2
2	E	271	VAL	2.1
2	F	271	VAL	2.1
1	C	392	GLU	2.1
2	F	162	VAL	2.1
2	F	295	GLN	2.1
1	A	139	GLN	2.1
2	E	1	PHE	2.1
2	D	203	PRO	2.1
2	E	251	GLU	2.1
1	B	123	PHE	2.1
2	E	317	PHE	2.1
2	D	62	ALA	2.1
1	A	211	PHE	2.1
1	A	188	VAL	2.0
2	E	298	LEU	2.0
2	E	183	ILE	2.0
2	D	295	GLN	2.0
2	D	207	MET	2.0
2	D	204	GLY	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.