



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:10 AM UTC

PDB ID : 8DN6 / pdb_00008dn6
Title : The crystal structure of the Arabidopsis thaliana Toc75 POTRA domains in complex with fab tc2
Authors : Srinivasan, K.; Noinaj, N.
Deposited on : 2022-07-10
Resolution : 3.00 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

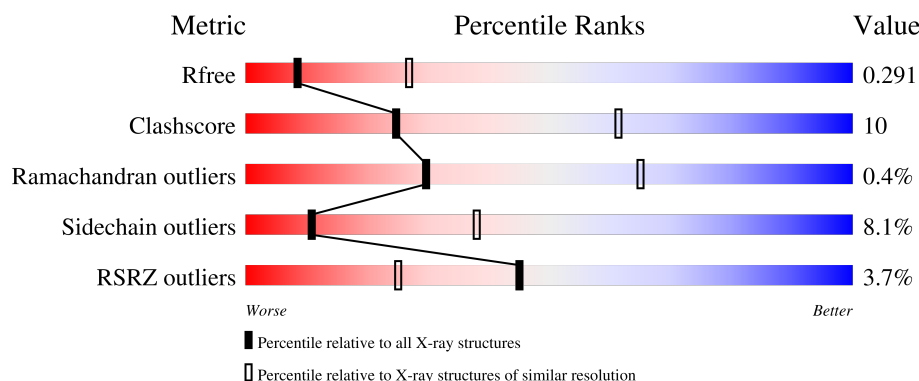
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	313	 4% 44% 16% • 37%
1	B	313	 3% 47% 15% • 37%
2	C	239	 4% 71% 21% • 7%
2	E	239	 4% 70% 21% • 8%
3	D	215	 % 75% 24%

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Mol	Chain	Length	Quality of chain
3	F	215	78% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9639 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 Protein TOC75-3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1566	982	283	292	9			
1	B	198	Total	C	N	O	S	0	0	0
			1565	982	281	294	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	expression tag	UNP Q9STE8
A	138	ALA	-	expression tag	UNP Q9STE8
A	139	MET	-	expression tag	UNP Q9STE8
A	140	GLY	-	expression tag	UNP Q9STE8
B	137	GLY	-	expression tag	UNP Q9STE8
B	138	ALA	-	expression tag	UNP Q9STE8
B	139	MET	-	expression tag	UNP Q9STE8
B	140	GLY	-	expression tag	UNP Q9STE8

- Molecule 2 is a protein called fabtc2_HC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1631	1038	267	321	5			
2	E	220	Total	C	N	O	S	0	1	0
			1635	1043	263	324	5			

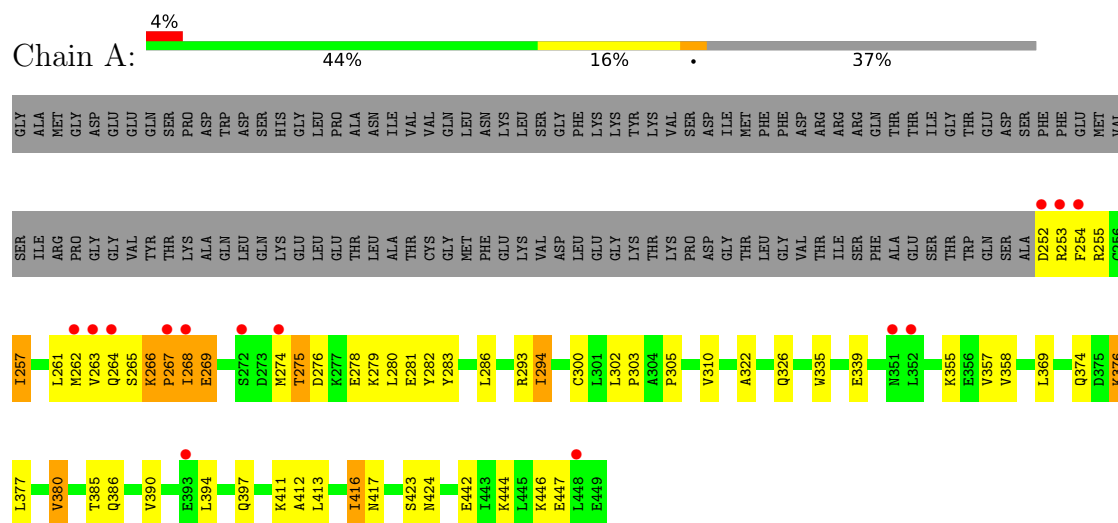
- Molecule 3 is a protein called fabtc2_LC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	0	0
			1619	1011	271	331	6			
3	F	215	Total	C	N	O	S	0	1	0
			1623	1013	271	333	6			

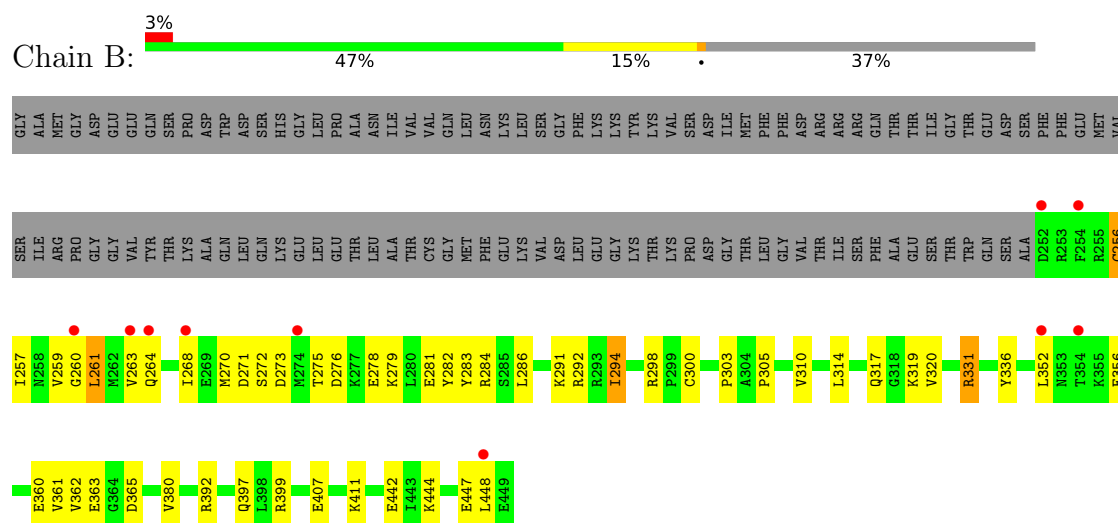
3 Residue-property plots

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

• Molecule 1: Protein TOC75-3, chloroplastic

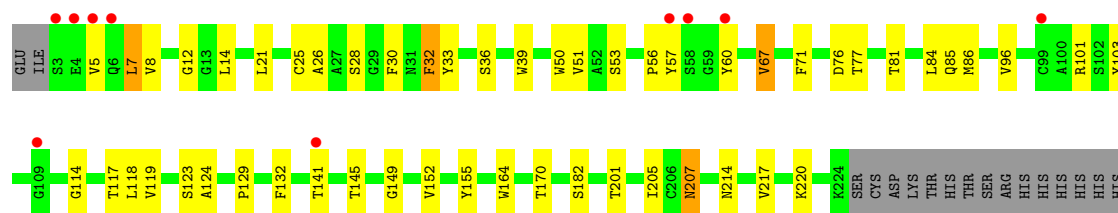


• Molecule 1: Protein TOC75-3, chloroplastic

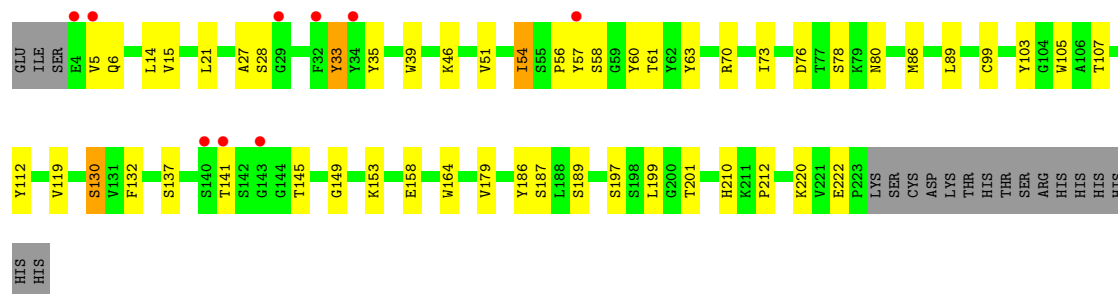


• Molecule 2: fabtc2_HC

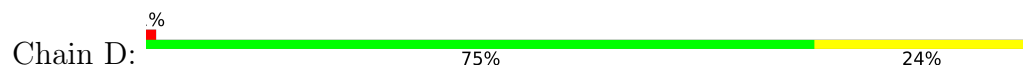




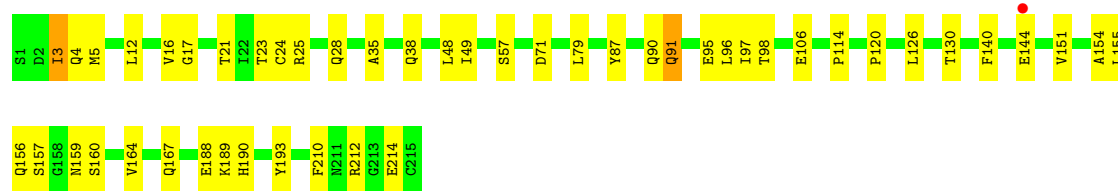
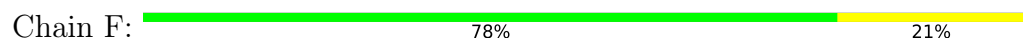
• Molecule 2: fabtc2_HC



• Molecule 3: fabtc2_LC



• Molecule 3: fabtc2_LC



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.09Å 51.48Å 172.08Å 90.00° 123.06° 90.00°	Depositor
Resolution (Å)	49.30 – 3.00 49.30 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.30-3.00) 99.3 (49.30-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.240 , 0.293 0.238 , 0.291	Depositor DCC
R_{free} test set	1991 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9639	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.27% 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	0.27	0/1587	0.59	0/2140
1	B	0.22	0/1587	0.50	0/2143
2	C	0.16	0/1677	0.49	0/2299
2	E	0.15	0/1684	0.50	0/2306
3	D	0.18	0/1655	0.48	0/2254
3	F	0.15	0/1662	0.46	0/2266
All	All	0.19	0/9852	0.51	0/13408

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	5	VAL	Peptide

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	1566	0	1576	37	0
1	B	1565	0	1558	36	0
2	C	1631	0	1537	34	0
2	E	1635	0	1550	31	0
3	D	1619	0	1530	34	0
3	F	1623	0	1532	24	0
All	All	9639	0	9283	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 10.

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)
3:D:19:ARG:HD3	3:D:77:SER:HA	1.26	1.11
3:D:19:ARG:CD	3:D:77:SER:HA	2.02	0.89
2:E:27:ALA:HB3	2:E:80:ASN:HB3	1.65	0.79
1:A:269:GLU:O	1:A:282:TYR:OH	2.02	0.77
1:A:276:ASP:OD2	2:C:101:ARG:NH1	2.22	0.71
1:A:376:LYS:HG3	1:A:377:LEU:HD22	1.72	0.71
2:E:76:ASP:OD1	2:E:78:SER:OG	2.07	0.70
3:F:90:GLN:HE21	3:F:97:ILE:HG23	1.56	0.70
1:A:274:MET:SD	3:D:57:SER:OG	2.48	0.70
2:C:7:LEU:HD11	2:C:25:CYS:SG	2.33	0.69
3:D:19:ARG:HH11	3:D:77:SER:N	1.91	0.68
3:D:90:GLN:HE21	3:D:97:ILE:HG23	1.57	0.68
3:F:154:ALA:O	3:F:156:GLN:NE2	2.25	0.68
1:A:442:GLU:OE2	1:A:444:LYS:HE3	1.95	0.65
2:E:6:GLN:H	2:E:28:SER:HB3	1.59	0.65
1:A:278:GLU:O	1:A:281:GLU:N	2.17	0.64
2:C:141:THR:HB	3:D:208:LYS:HE3	1.78	0.64
2:E:54:ILE:HG22	2:E:61:THR:HG22	1.81	0.63
1:B:279:LYS:NZ	2:E:112:TYR:OH	2.33	0.61
1:A:413:LEU:O	1:A:417:ASN:HB2	2.01	0.61
1:B:261:LEU:HD22	1:B:263:VAL:H	1.67	0.60
2:E:6:GLN:HG2	2:E:28:SER:HB2	1.84	0.60
1:A:424:ASN:HB3	1:A:446:LYS:HB3	1.84	0.60
1:B:257:ILE:HD13	1:B:310:VAL:HG11	1.83	0.59
1:B:263:VAL:HG11	1:B:365:ASP:OD1	2.01	0.59
1:A:386:GLN:NE2	1:A:447:GLU:OE2	2.22	0.59
2:C:86:MET:HE1	2:C:119:VAL:HG11	1.85	0.58
3:D:19:ARG:HA	3:D:76:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:PHE:CE1	2:C:32:PHE:HB3	2.38	0.58
1:B:270:MET:HE3	1:B:271:ASP:H	1.69	0.58
1:B:303:PRO:HB2	1:B:305:PRO:HD2	1.86	0.57
1:B:278:GLU:O	1:B:281:GLU:N	2.38	0.57
1:B:298:ARG:NH2	1:B:363:GLU:OE1	2.37	0.57
1:B:261:LEU:HD11	1:B:298:ARG:HE	1.68	0.57
1:B:263:VAL:HG23	1:B:362:VAL:HA	1.87	0.56
2:C:50:TRP:NE1	2:C:53:SER:OG	2.34	0.56
2:C:149:GLY:HA2	2:C:164:TRP:CZ2	2.41	0.56
1:B:283:TYR:HB3	2:E:103:TYR:CD2	2.41	0.56
1:B:261:LEU:CD1	1:B:298:ARG:HE	2.18	0.55
2:E:158:GLU:HG3	2:E:186:TYR:CE2	2.42	0.54
2:C:71:PHE:HA	2:C:85:GLN:O	2.06	0.54
3:F:3:ILE:HD13	3:F:91:GLN:HE21	1.72	0.54
2:C:39:TRP:O	2:C:51:VAL:HG12	2.07	0.54
3:F:188:GLU:O	3:F:212:ARG:NH2	2.40	0.54
2:E:33:TYR:CD1	2:E:56:PRO:HB3	2.43	0.53
1:A:278:GLU:O	1:A:281:GLU:HG3	2.08	0.53
1:B:261:LEU:HD11	1:B:298:ARG:NE	2.23	0.53
1:A:385:THR:HG23	1:A:386:GLN:HG3	1.91	0.52
1:B:261:LEU:HD13	1:B:261:LEU:O	2.09	0.52
2:C:7:LEU:HD13	2:C:8:VAL:N	2.24	0.52
3:D:154:ALA:O	3:D:156:GLN:NE2	2.38	0.52
3:F:3:ILE:HD13	3:F:91:GLN:NE2	2.25	0.52
3:F:120:PRO:HB3	3:F:210:PHE:CE2	2.45	0.52
1:A:274:MET:SD	1:A:274:MET:N	2.83	0.51
1:A:262:MET:HE2	1:A:293:ARG:CZ	2.40	0.51
1:B:261:LEU:CD1	1:B:298:ARG:HB3	2.40	0.51
3:F:35:ALA:HA	3:F:49:ILE:O	2.10	0.51
2:C:30:PHE:HE1	2:C:32:PHE:HB3	1.76	0.50
3:F:114:PRO:HB3	3:F:140:PHE:CD2	2.47	0.50
3:D:194:ALA:HB2	3:D:209:SER:HB3	1.92	0.50
1:B:260:GLY:O	1:B:360:GLU:HA	2.12	0.50
2:C:71:PHE:CE2	2:C:86:MET:HG2	2.46	0.50
3:D:190:HIS:O	3:D:212:ARG:HD3	2.12	0.50
2:C:67:VAL:HG13	2:C:71:PHE:HB2	1.93	0.50
2:E:130:SER:HB2	2:E:132:PHE:CE1	2.46	0.50
3:F:106:GLU:HB2	3:F:167:GLN:OE1	2.11	0.50
2:E:33:TYR:HD1	2:E:56:PRO:HB3	1.77	0.49
3:F:151:VAL:H	3:F:156:GLN:NE2	2.10	0.49
3:D:19:ARG:HD2	3:D:76:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:210:HIS:CD2	2:E:212:PRO:HD2	2.47	0.49
2:C:36:SER:HB3	2:C:56:PRO:HD3	1.95	0.49
2:E:86:MET:HE1	2:E:119:VAL:HG11	1.93	0.49
1:B:291:LYS:O	1:B:294:ILE:HG13	2.12	0.49
1:A:275:THR:OG1	1:A:278:GLU:HB3	2.13	0.48
3:F:159:ASN:OD1	3:F:159:ASN:N	2.46	0.48
1:A:278:GLU:OE2	1:A:279:LYS:HD3	2.12	0.48
1:A:397:GLN:H	1:A:397:GLN:CD	2.21	0.48
1:A:423:SER:N	1:A:446:LYS:O	2.47	0.48
1:B:273:ASP:O	3:F:57:SER:HB2	2.13	0.48
3:D:5:MET:HE2	3:D:91:GLN:HB2	1.96	0.48
2:C:7:LEU:HB3	2:C:114:GLY:HA2	1.96	0.47
3:D:19:ARG:HH11	3:D:77:SER:CA	2.27	0.47
3:D:119:PHE:HB2	3:D:134:VAL:HB	1.96	0.47
2:C:96:VAL:HG22	2:C:118:LEU:HD12	1.96	0.47
3:D:114:PRO:HB3	3:D:140:PHE:HB3	1.96	0.47
2:C:12:GLY:HA2	2:C:21:LEU:HD21	1.97	0.47
2:E:33:TYR:O	2:E:56:PRO:HB2	2.14	0.47
1:B:442:GLU:OE2	1:B:444:LYS:HE2	2.14	0.47
2:E:63:TYR:CE2	2:E:73:ILE:HG22	2.50	0.47
1:B:276:ASP:OD1	1:B:276:ASP:C	2.57	0.47
1:A:252:ASP:HA	2:C:60:TYR:OH	2.15	0.46
2:C:25:CYS:HB2	2:C:39:TRP:CH2	2.49	0.46
1:B:319:LYS:HZ3	2:E:60:TYR:HD2	1.62	0.46
2:C:76:ASP:HB3	2:C:81:THR:OG1	2.15	0.46
1:B:282:TYR:O	1:B:286:LEU:HG	2.16	0.46
3:F:193:TYR:HB2	3:F:210:PHE:CE1	2.50	0.46
2:C:14:LEU:HD21	2:C:124:ALA:HB3	1.98	0.46
3:D:82:GLU:OE1	3:D:82:GLU:N	2.35	0.46
2:E:158:GLU:HG3	2:E:186:TYR:CD2	2.51	0.46
1:B:275:THR:HG22	1:B:276:ASP:H	1.81	0.46
3:D:171:ASP:OD1	3:D:171:ASP:C	2.58	0.46
2:E:220:LYS:HE2	2:E:222:GLU:OE1	2.16	0.46
3:F:95:GLU:HG2	3:F:96:LEU:N	2.31	0.46
1:A:411:LYS:HA	1:A:411:LYS:HD2	1.77	0.45
1:B:275:THR:HG22	1:B:276:ASP:N	2.30	0.45
1:A:279:LYS:HD3	1:A:279:LYS:HA	1.76	0.45
1:B:259:VAL:HG12	1:B:300:CYS:SG	2.56	0.45
2:E:35:TYR:O	2:E:56:PRO:HD2	2.16	0.45
3:D:202:LEU:HD13	3:D:206:VAL:HG13	1.98	0.45
3:D:49:ILE:HG22	3:D:51:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:15:VAL:HG11	2:E:21:LEU:HB2	1.99	0.45
2:E:153:LYS:O	2:E:187:SER:HB2	2.16	0.45
1:B:261:LEU:HD12	1:B:298:ARG:HB3	1.99	0.45
1:A:335:TRP:CZ2	1:A:339:GLU:HG3	2.52	0.45
3:F:38:GLN:HB2	3:F:87:TYR:CE1	2.52	0.45
2:C:149:GLY:HA2	2:C:164:TRP:CH2	2.52	0.45
3:D:114:PRO:HB3	3:D:140:PHE:CD2	2.52	0.44
3:D:95:GLU:HG2	3:D:96:LEU:N	2.31	0.44
2:C:129:PRO:HB2	2:C:152:VAL:HG13	2.00	0.44
2:C:205:ILE:HG12	2:C:220:LYS:HA	2.00	0.44
2:E:56:PRO:C	2:E:58:SER:H	2.25	0.44
2:E:199:LEU:HD23	2:E:199:LEU:HA	1.84	0.44
2:E:39:TRP:HD1	2:E:73:ILE:HD12	1.83	0.44
1:A:303:PRO:HB2	1:A:305:PRO:HD2	2.00	0.44
2:C:132:PHE:CE2	3:D:125:GLN:HG3	2.52	0.44
3:D:171:ASP:OD1	3:D:173:THR:HG22	2.17	0.44
3:D:19:ARG:HD2	3:D:76:ILE:C	2.42	0.44
1:A:283:TYR:HB3	2:C:103:TYR:CD1	2.53	0.43
2:E:54:ILE:HA	2:E:60:TYR:O	2.18	0.43
3:F:155:LEU:HD23	3:F:157[A]:SER:H	1.83	0.43
1:B:270:MET:HE3	1:B:271:ASP:N	2.32	0.43
1:A:300:CYS:SG	1:A:302:LEU:HB2	2.59	0.43
1:A:374:GLN:HA	1:A:380:VAL:HA	2.00	0.43
1:B:319:LYS:NZ	2:E:60:TYR:HD2	2.17	0.43
2:E:141:THR:HG22	2:E:197:SER:HA	2.01	0.43
3:F:48:LEU:C	3:F:49:ILE:HD12	2.43	0.43
1:A:257:ILE:HD13	1:A:310:VAL:HG11	2.00	0.43
1:A:416:ILE:HG13	1:A:417:ASN:N	2.30	0.43
3:F:5:MET:HE3	3:F:24:CYS:SG	2.59	0.43
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.79	0.43
3:F:17:GLY:N	3:F:79:LEU:O	2.51	0.43
1:A:282:TYR:O	1:A:286:LEU:HG	2.17	0.43
1:B:392:ARG:HD2	1:B:392:ARG:HA	1.76	0.43
2:E:149:GLY:HA2	2:E:164:TRP:CZ2	2.54	0.43
3:F:4:GLN:HA	3:F:98:THR:HG21	2.00	0.43
3:D:184:LYS:O	3:D:188:GLU:HG2	2.19	0.42
3:F:25:ARG:HB2	3:F:71:ASP:OD1	2.19	0.42
1:B:331:ARG:HA	1:B:331:ARG:HD2	1.64	0.42
2:E:86:MET:HE2	2:E:89:LEU:HD11	2.02	0.42
1:A:253:ARG:HG2	1:A:254:PHE:H	1.84	0.42
3:D:159:ASN:OD1	3:D:159:ASN:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:PHE:CZ	2:C:77:THR:HA	2.54	0.42
2:C:7:LEU:HD21	2:C:25:CYS:SG	2.59	0.42
2:C:207:ASN:N	2:C:207:ASN:OD1	2.52	0.42
3:F:155:LEU:HD23	3:F:157[B]:SER:H	1.83	0.42
1:A:322:ALA:O	1:A:326:GLN:HG3	2.20	0.42
3:D:90:GLN:HA	3:D:98:THR:O	2.20	0.41
3:D:116:VAL:O	3:D:208:LYS:HE2	2.20	0.41
1:A:294:ILE:HD12	1:A:294:ILE:HA	1.83	0.41
1:B:261:LEU:HD13	1:B:261:LEU:C	2.45	0.41
1:B:397:GLN:OE1	1:B:397:GLN:N	2.45	0.41
2:C:76:ASP:HB3	2:C:81:THR:HG1	1.84	0.41
1:A:412:ALA:O	1:A:416:ILE:HG23	2.19	0.41
1:B:352:LEU:HB2	1:B:356:GLU:OE1	2.19	0.41
1:A:390:VAL:O	1:A:394:LEU:HG	2.20	0.41
2:C:7:LEU:HD22	2:C:26:ALA:O	2.20	0.41
3:D:19:ARG:NH1	3:D:77:SER:HB3	2.35	0.41
1:A:267:PRO:O	1:A:268:ILE:HB	2.20	0.41
2:C:67:VAL:HG22	2:C:71:PHE:CD1	2.55	0.41
3:F:190:HIS:O	3:F:212:ARG:NH2	2.47	0.41
2:E:105:TRP:O	2:E:107:THR:HG22	2.20	0.41
1:A:294:ILE:HD11	1:A:358:VAL:HG11	2.03	0.41
2:E:33:TYR:HB3	2:E:57:TYR:CE2	2.56	0.41
2:C:71:PHE:HD2	2:C:84:LEU:HD11	1.86	0.41
3:F:189:LYS:O	3:F:190:HIS:CG	2.74	0.41
3:D:34:VAL:HA	3:D:90:GLN:O	2.21	0.41
2:C:129:PRO:HB3	2:C:155:TYR:HB3	2.02	0.40
1:A:266:LYS:HA	1:A:267:PRO:HD3	1.93	0.40
3:D:118:ILE:HD12	3:D:118:ILE:HA	1.90	0.40
1:B:300:CYS:HB3	1:B:336:TYR:OH	2.21	0.40
3:D:19:ARG:CZ	3:D:75:THR:HG22	2.51	0.40
3:D:109:ARG:HD3	3:D:110:THR:O	2.21	0.40
1:A:255:ARG:N	1:A:355:LYS:O	2.51	0.40
1:B:256:CYS:SG	1:B:356:GLU:HG3	2.61	0.40
3:D:125:GLN:HG2	3:D:130:THR:O	2.21	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	196/313 (63%)	182 (93%)	10 (5%)	4 (2%)	6	28
1	B	196/313 (63%)	186 (95%)	10 (5%)	0	100	100
2	C	220/239 (92%)	205 (93%)	14 (6%)	1 (0%)	24	60
2	E	219/239 (92%)	202 (92%)	17 (8%)	0	100	100
3	D	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
3	F	214/215 (100%)	205 (96%)	9 (4%)	0	100	100
All	All	1257/1534 (82%)	1183 (94%)	69 (6%)	5 (0%)	30	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	267	PRO
1	A	268	ILE
1	A	269	GLU
2	C	57	TYR

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	170/276 (62%)	157 (92%)	13 (8%)	12	41
1	B	169/276 (61%)	151 (89%)	18 (11%)	6	26
2	C	174/200 (87%)	160 (92%)	14 (8%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	176/200 (88%)	162 (92%)	14 (8%)	11	38
3	D	182/190 (96%)	169 (93%)	13 (7%)	13	43
3	F	183/190 (96%)	170 (93%)	13 (7%)	13	43
All	All	1054/1332 (79%)	969 (92%)	85 (8%)	11	38

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ILE
1	A	261	LEU
1	A	263	VAL
1	A	265	SER
1	A	266	LYS
1	A	275	THR
1	A	280	LEU
1	A	294	ILE
1	A	357	VAL
1	A	369	LEU
1	A	376	LYS
1	A	380	VAL
1	A	416	ILE
1	B	256	CYS
1	B	261	LEU
1	B	264	GLN
1	B	268	ILE
1	B	272	SER
1	B	284	ARG
1	B	292	ARG
1	B	294	ILE
1	B	317	GLN
1	B	320	VAL
1	B	331	ARG
1	B	361	VAL
1	B	380	VAL
1	B	399	ARG
1	B	407	GLU
1	B	411	LYS
1	B	447	GLU
1	B	448	LEU
2	C	7	LEU
2	C	28	SER

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Mol	Chain	Res	Type
2	C	32	PHE
2	C	33	TYR
2	C	67	VAL
2	C	117	THR
2	C	123	SER
2	C	145	THR
2	C	170	THR
2	C	182	SER
2	C	201	THR
2	C	207	ASN
2	C	214	ASN
2	C	217	VAL
3	D	2	ASP
3	D	3	ILE
3	D	4	GLN
3	D	20	VAL
3	D	64	SER
3	D	94	TRP
3	D	160	SER
3	D	165	THR
3	D	181	THR
3	D	198	THR
3	D	203	SER
3	D	209	SER
3	D	214	GLU
2	E	5	VAL
2	E	14	LEU
2	E	33	TYR
2	E	46	LYS
2	E	51	VAL
2	E	54	ILE
2	E	70	ARG
2	E	99	CYS
2	E	130	SER
2	E	137	SER
2	E	145	THR
2	E	179	VAL
2	E	189	SER
2	E	201	THR
3	F	3	ILE
3	F	12	LEU
3	F	16	VAL

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Mol	Chain	Res	Type
3	F	21	THR
3	F	23	THR
3	F	28	GLN
3	F	91	GLN
3	F	126	LEU
3	F	130	THR
3	F	144	GLU
3	F	160	SER
3	F	164	VAL
3	F	214	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	384	ASN
1	A	424	ASN
1	B	372	GLN
1	B	374	GLN
1	B	400	GLN
1	B	435	ASN
3	D	90	GLN
3	D	190	HIS
3	F	90	GLN
3	F	91	GLN
3	F	138	ASN
3	F	156	GLN

5.3.3 RNA [i](#)

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

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, 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	198/313 (63%)	0.41	14 (7%)	22 11	36, 66, 127, 176	0
1	B	198/313 (63%)	0.33	10 (5%)	33 17	24, 63, 115, 142	0
2	C	222/239 (92%)	0.52	10 (4%)	38 20	48, 82, 133, 197	0
2	E	220/239 (92%)	0.36	9 (4%)	41 23	46, 75, 126, 204	1 (0%)
3	D	214/215 (99%)	0.25	3 (1%)	73 51	48, 71, 118, 141	0
3	F	215/215 (100%)	0.16	1 (0%)	87 72	43, 69, 120, 137	1 (0%)
All	All	1267/1534 (82%)	0.34	47 (3%)	45 25	24, 72, 125, 204	2 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	MET	4.8
1	A	252	ASP	4.6
1	A	352	LEU	3.3
2	C	5	VAL	3.2
2	C	141	THR	3.2
2	E	57	TYR	3.1
2	E	141	THR	3.1
1	A	253	ARG	3.0
1	B	354	THR	3.0
2	C	4	GLU	2.9
2	C	6	GLN	2.9
1	A	351	ASN	2.9
2	E	4	GLU	2.8
2	E	143	GLY	2.8
1	B	263	VAL	2.8
1	B	254	PHE	2.7
1	A	263	VAL	2.6
1	A	274	MET	2.6
2	C	57	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	254	PHE	2.5
1	A	393	GLU	2.5
1	A	268	ILE	2.5
1	B	268	ILE	2.5
2	C	3	SER	2.5
2	C	99	CYS	2.4
2	E	34	TYR	2.4
3	D	19	ARG	2.4
1	B	264	GLN	2.4
1	B	352	LEU	2.4
3	D	3	ILE	2.3
1	A	448	LEU	2.3
2	E	32	PHE	2.3
3	D	155	LEU	2.3
1	B	260	GLY	2.3
1	A	267	PRO	2.2
3	F	144	GLU	2.2
2	E	29	GLY	2.2
1	A	272	SER	2.2
2	C	60	TYR	2.1
2	E	140	SER	2.1
2	E	5	VAL	2.1
1	B	448	LEU	2.1
1	B	274	MET	2.0
2	C	109	GLY	2.0
2	C	58	SER	2.0
1	B	252	ASP	2.0
1	A	264	GLN	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 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.