



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:31 AM UTC

PDB ID : 2ZQP / pdb_00002zqp
Title : Crystal Structure of SecYE translocon from *Thermus thermophilus*
Authors : Tsukazaki, T.; Nureki, O.
Deposited on : 2008-08-14
Resolution : 6.00 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

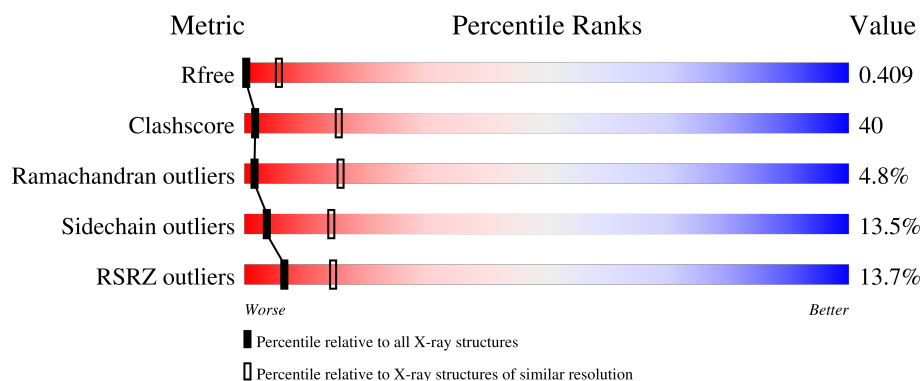
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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	Y	434	14% 41% 43% 10% ••
2	E	60	5% 28% 40% 8% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3594 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 Preprotein translocase SecY subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	415	Total	C	N	O	S	0	0	0
			3226	2155	529	536	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	2	VAL	LEU	engineered mutation	UNP Q8KZP3
Y	252	GLY	ARG	engineered mutation	UNP Q8KZP3

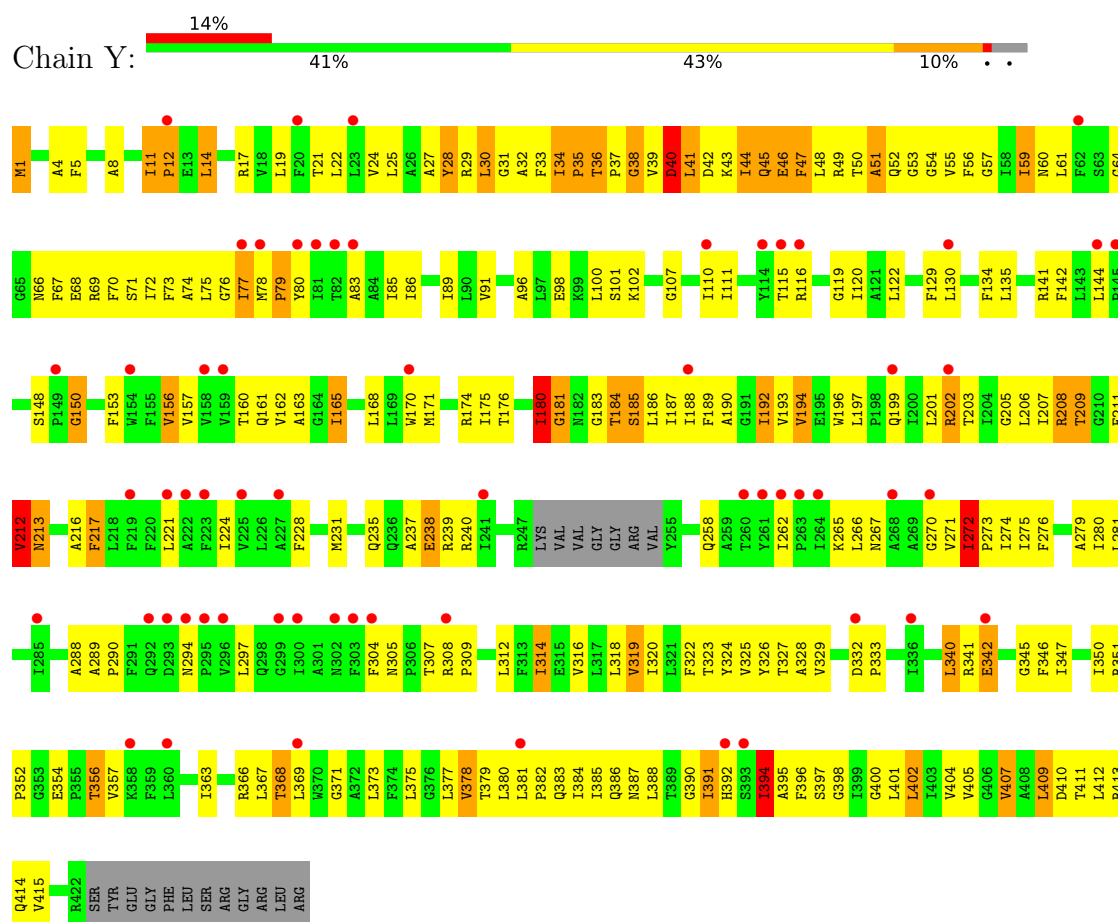
- Molecule 2 is a protein called Preprotein translocase SecE subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	46	Total	C	N	O	S	0	0	0
			368	245	61	61	1			

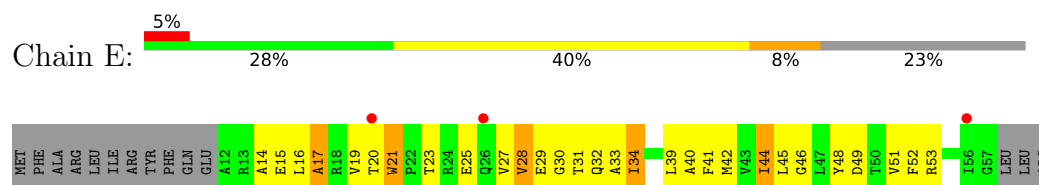
3 Residue-property plots [i](#)

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: Preprotein translocase SecY subunit



• Molecule 2: Preprotein translocase SecE subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.88Å 91.88Å 240.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.92 – 6.00 42.92 – 6.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (42.92-6.00) 93.8 (42.92-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 6.14Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.407 , 0.445 0.413 , 0.409	Depositor DCC
R_{free} test set	123 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	339.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 877.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	3594	wwPDB-VP
Average B, all atoms (Å ²)	368.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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	Y	0.69	0/3305	1.08	21/4499 (0.5%)
2	E	0.71	0/375	1.01	0/510
All	All	0.70	0/3680	1.07	21/5009 (0.4%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	34	ILE	N-CA-C	7.95	114.79	107.56
1	Y	308	ARG	CA-C-N	7.52	129.24	119.84
1	Y	308	ARG	C-N-CA	7.52	129.24	119.84
1	Y	202	ARG	N-CA-C	-7.09	103.48	111.14
1	Y	180	ILE	CB-CA-C	-6.80	104.11	111.59
1	Y	44	ILE	N-CA-C	6.70	118.04	111.67
1	Y	47	PHE	N-CA-C	-6.62	104.15	111.36
1	Y	272	ILE	CB-CA-C	-6.18	107.82	113.70
1	Y	36	THR	CA-C-N	6.13	127.50	119.84
1	Y	36	THR	C-N-CA	6.13	127.50	119.84
1	Y	150	GLY	CA-C-N	6.05	125.77	119.05
1	Y	150	GLY	C-N-CA	6.05	125.77	119.05
1	Y	11	ILE	CA-C-N	5.44	126.64	119.84
1	Y	11	ILE	C-N-CA	5.44	126.64	119.84
1	Y	327	THR	N-CA-C	-5.35	107.05	113.21
1	Y	363	ILE	N-CA-C	5.33	115.99	110.82
1	Y	41	LEU	N-CA-C	-5.32	99.46	110.80
1	Y	40	ASP	N-CA-C	-5.28	99.56	110.80
1	Y	356	THR	N-CA-C	-5.21	107.10	113.50
1	Y	163	ALA	N-CA-C	-5.15	106.23	112.88
1	Y	346	PHE	N-CA-C	5.11	116.29	108.52

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	Y	3226	0	3373	274	3
2	E	368	0	384	49	0
All	All	3594	0	3757	296	3

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 40.

All (296) 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:Y:206:LEU:HB3	1:Y:211:GLU:CB	1.70	1.21
1:Y:206:LEU:CB	1:Y:211:GLU:HB2	1.76	1.15
1:Y:366:ARG:HB3	2:E:14:ALA:HB2	1.26	1.14
1:Y:192:ILE:HG21	1:Y:400:GLY:HA3	1.18	1.14
1:Y:17:ARG:HB3	1:Y:180:ILE:HG23	1.26	1.13
1:Y:17:ARG:CB	1:Y:180:ILE:HG23	1.80	1.12
1:Y:212:VAL:HG13	1:Y:213:ASN:H	1.07	1.12
1:Y:46:GLU:HA	1:Y:49:ARG:HB2	1.40	1.03
1:Y:50:THR:HB	1:Y:52:GLN:OE1	1.60	1.02
1:Y:202:ARG:O	1:Y:206:LEU:HG	1.60	1.01
1:Y:40:ASP:OD2	1:Y:42:ASP:HB2	1.61	1.00
1:Y:192:ILE:HG21	1:Y:400:GLY:CA	1.91	0.99
1:Y:32:ALA:HA	1:Y:66:ASN:OD1	1.63	0.96
1:Y:206:LEU:HB3	1:Y:211:GLU:HB2	0.90	0.90
1:Y:35:PRO:HB3	1:Y:41:LEU:HD13	1.54	0.88
1:Y:383:GLN:HE22	1:Y:392:HIS:HE1	1.20	0.88
1:Y:212:VAL:HG13	1:Y:213:ASN:N	1.86	0.88
1:Y:46:GLU:HA	1:Y:49:ARG:CB	2.05	0.86
1:Y:40:ASP:O	1:Y:43:LYS:N	2.08	0.85
1:Y:386:GLN:HG2	1:Y:391:ILE:O	1.78	0.84
1:Y:78:MET:HB2	1:Y:79:PRO:HD3	1.59	0.83
1:Y:129:PHE:CE1	1:Y:290:PRO:HG2	2.14	0.82
1:Y:46:GLU:HG2	1:Y:46:GLU:O	1.78	0.82
1:Y:192:ILE:CG2	1:Y:400:GLY:HA3	2.06	0.82
1:Y:383:GLN:HE22	1:Y:392:HIS:CE1	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:183:GLY:O	1:Y:187:ILE:HG12	1.80	0.81
1:Y:202:ARG:HG2	1:Y:206:LEU:HD11	1.61	0.80
1:Y:45:GLN:O	1:Y:48:LEU:N	2.15	0.79
1:Y:189:PHE:HE1	1:Y:404:VAL:HA	1.47	0.79
1:Y:275:ILE:HG13	1:Y:276:PHE:H	1.47	0.79
1:Y:53:GLY:O	1:Y:56:PHE:HB2	1.83	0.78
1:Y:221:LEU:HD23	1:Y:224:ILE:HD12	1.66	0.77
1:Y:50:THR:O	1:Y:54:GLY:N	2.16	0.77
1:Y:17:ARG:HB2	1:Y:180:ILE:HG23	1.64	0.76
1:Y:44:ILE:CD1	1:Y:135:LEU:HD21	2.15	0.76
1:Y:184:THR:O	1:Y:186:LEU:N	2.17	0.76
1:Y:196:TRP:CZ3	1:Y:401:LEU:HD13	2.21	0.76
1:Y:85:ILE:O	1:Y:89:ILE:HG13	1.85	0.75
1:Y:50:THR:CB	1:Y:52:GLN:OE1	2.34	0.75
1:Y:28:TYR:HB2	1:Y:171:MET:SD	2.27	0.74
1:Y:274:ILE:HD12	1:Y:319:VAL:HG13	1.69	0.74
1:Y:231:MET:O	1:Y:235:GLN:HG2	1.88	0.74
1:Y:129:PHE:HE1	1:Y:290:PRO:HG2	1.54	0.73
2:E:16:LEU:HA	2:E:19:VAL:HG21	1.70	0.73
1:Y:29:ARG:HG2	2:E:48:TYR:HB2	1.70	0.73
1:Y:41:LEU:CD1	1:Y:69:ARG:O	2.37	0.73
1:Y:41:LEU:O	1:Y:44:ILE:HG22	1.89	0.73
1:Y:46:GLU:O	1:Y:50:THR:CG2	2.36	0.73
1:Y:40:ASP:HB3	1:Y:43:LYS:HB2	1.71	0.73
1:Y:35:PRO:CB	1:Y:41:LEU:HD13	2.19	0.72
1:Y:41:LEU:HD11	1:Y:69:ARG:O	1.88	0.72
1:Y:199:GLN:OE1	1:Y:396:PHE:HE2	1.72	0.72
1:Y:212:VAL:CG1	1:Y:213:ASN:H	1.92	0.72
1:Y:316:VAL:O	1:Y:320:ILE:HG13	1.89	0.72
1:Y:46:GLU:CA	1:Y:49:ARG:HB2	2.18	0.70
1:Y:275:ILE:HG13	1:Y:276:PHE:N	2.05	0.70
1:Y:382:PRO:HA	1:Y:385:ILE:HB	1.73	0.70
1:Y:44:ILE:HG12	1:Y:70:PHE:HB2	1.74	0.69
1:Y:304:PHE:CE1	1:Y:314:ILE:HG21	2.28	0.69
1:Y:17:ARG:HB3	1:Y:180:ILE:CG2	2.14	0.68
1:Y:273:PRO:CB	1:Y:323:THR:HA	2.25	0.67
1:Y:273:PRO:HB2	1:Y:323:THR:HA	1.76	0.66
2:E:20:THR:C	2:E:21:TRP:HD1	2.02	0.66
1:Y:267:ASN:HD21	1:Y:323:THR:HG21	1.61	0.66
1:Y:100:LEU:O	1:Y:107:GLY:HA3	1.95	0.65
1:Y:239:ARG:HA	2:E:19:VAL:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:213:ASN:O	1:Y:217:PHE:HB2	1.97	0.65
1:Y:412:LEU:HD13	2:E:33:ALA:HB1	1.78	0.65
2:E:48:TYR:HB3	2:E:52:PHE:CE1	2.32	0.65
1:Y:190:ALA:HB2	2:E:41:PHE:CE1	2.31	0.64
2:E:21:TRP:C	2:E:23:THR:H	2.03	0.64
1:Y:28:TYR:O	1:Y:73:PHE:HE1	1.81	0.63
1:Y:39:VAL:O	1:Y:41:LEU:N	2.31	0.63
1:Y:189:PHE:CE1	1:Y:404:VAL:HA	2.30	0.63
2:E:44:ILE:HG23	2:E:48:TYR:OH	1.99	0.63
1:Y:153:PHE:O	1:Y:157:VAL:HG23	1.99	0.62
1:Y:375:LEU:HA	1:Y:378:VAL:HB	1.81	0.62
1:Y:196:TRP:CH2	1:Y:401:LEU:HB2	2.34	0.62
1:Y:332:ASP:HB2	1:Y:333:PRO:HD3	1.81	0.62
1:Y:45:GLN:HB3	1:Y:68:GLU:HG2	1.82	0.62
1:Y:66:ASN:OD1	1:Y:73:PHE:HB2	1.99	0.62
1:Y:141:ARG:HD3	1:Y:142:PHE:CE1	2.34	0.62
1:Y:193:VAL:HG12	1:Y:404:VAL:HG22	1.83	0.61
1:Y:206:LEU:CA	1:Y:211:GLU:HB2	2.30	0.61
1:Y:206:LEU:HA	1:Y:209:THR:OG1	2.01	0.61
1:Y:194:VAL:HB	2:E:45:LEU:HD13	1.83	0.61
1:Y:75:LEU:O	1:Y:78:MET:HG2	2.00	0.61
1:Y:40:ASP:OD2	1:Y:42:ASP:CB	2.43	0.60
1:Y:86:ILE:HA	1:Y:89:ILE:HD12	1.83	0.60
1:Y:134:PHE:CE2	1:Y:142:PHE:CZ	2.89	0.60
1:Y:202:ARG:C	1:Y:206:LEU:HG	2.26	0.60
1:Y:190:ALA:HA	1:Y:193:VAL:HG22	1.83	0.60
1:Y:384:ILE:O	1:Y:388:LEU:HG	2.01	0.60
2:E:21:TRP:CD1	2:E:21:TRP:N	2.69	0.59
1:Y:47:PHE:C	1:Y:47:PHE:CD2	2.80	0.59
1:Y:85:ILE:O	1:Y:89:ILE:N	2.35	0.59
1:Y:206:LEU:HD22	1:Y:211:GLU:CD	2.28	0.58
1:Y:239:ARG:HD2	2:E:19:VAL:HG22	1.85	0.58
1:Y:17:ARG:O	1:Y:180:ILE:HG12	2.02	0.58
1:Y:44:ILE:HD12	1:Y:135:LEU:HD21	1.83	0.58
1:Y:280:ILE:HB	1:Y:318:LEU:HD21	1.83	0.58
1:Y:400:GLY:O	1:Y:404:VAL:HG23	2.03	0.57
1:Y:40:ASP:O	1:Y:41:LEU:C	2.48	0.57
1:Y:239:ARG:HB2	2:E:19:VAL:HG22	1.87	0.57
1:Y:351:ARG:O	1:Y:356:THR:OG1	2.23	0.57
1:Y:235:GLN:O	1:Y:265:LYS:HE3	2.05	0.57
1:Y:35:PRO:HB3	1:Y:41:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:MET:O	2:E:46:GLY:N	2.35	0.57
1:Y:45:GLN:O	1:Y:47:PHE:N	2.38	0.56
1:Y:212:VAL:CG1	1:Y:213:ASN:N	2.56	0.56
1:Y:46:GLU:O	1:Y:50:THR:HG23	2.04	0.56
1:Y:203:THR:O	1:Y:207:ILE:HG13	2.04	0.56
1:Y:98:GLU:O	1:Y:102:LYS:N	2.40	0.55
1:Y:148:SER:C	1:Y:150:GLY:H	2.13	0.55
1:Y:193:VAL:HB	2:E:42:MET:HG2	1.88	0.55
1:Y:71:SER:O	1:Y:74:ALA:HB2	2.06	0.55
1:Y:304:PHE:HE1	1:Y:314:ILE:HG21	1.70	0.55
1:Y:130:LEU:O	1:Y:134:PHE:HB3	2.07	0.55
1:Y:60:ASN:HA	1:Y:67:PHE:HB3	1.89	0.55
1:Y:83:ALA:HB2	1:Y:122:LEU:HD11	1.89	0.55
1:Y:267:ASN:HD21	1:Y:323:THR:CG2	2.20	0.55
1:Y:192:ILE:HD13	1:Y:400:GLY:HA2	1.88	0.54
1:Y:55:VAL:C	1:Y:57:GLY:H	2.15	0.54
1:Y:316:VAL:HG12	1:Y:320:ILE:HD11	1.89	0.54
1:Y:35:PRO:CA	1:Y:41:LEU:HD13	2.37	0.54
1:Y:41:LEU:HD12	1:Y:69:ARG:O	2.06	0.54
1:Y:77:ILE:O	1:Y:77:ILE:HG13	2.07	0.54
2:E:21:TRP:C	2:E:23:THR:N	2.64	0.54
2:E:30:GLY:O	2:E:34:ILE:HG13	2.08	0.53
1:Y:34:ILE:O	1:Y:71:SER:HA	2.08	0.53
1:Y:64:GLY:O	1:Y:69:ARG:NH2	2.42	0.53
1:Y:307:THR:HG22	1:Y:397:SER:HB3	1.89	0.53
1:Y:312:LEU:HD21	1:Y:380:LEU:O	2.09	0.53
1:Y:22:LEU:HA	1:Y:25:LEU:HB2	1.90	0.53
1:Y:29:ARG:NE	1:Y:194:VAL:HG21	2.24	0.53
2:E:20:THR:C	2:E:21:TRP:CD1	2.85	0.53
2:E:21:TRP:HD1	2:E:21:TRP:N	2.07	0.53
1:Y:212:VAL:C	1:Y:213:ASN:CG	2.75	0.52
1:Y:51:ALA:C	1:Y:52:GLN:HG3	2.34	0.52
1:Y:46:GLU:HA	1:Y:49:ARG:CG	2.39	0.52
1:Y:240:ARG:HD2	2:E:20:THR:HB	1.92	0.52
1:Y:19:LEU:HA	1:Y:22:LEU:HD12	1.92	0.52
1:Y:35:PRO:HB3	1:Y:41:LEU:CD1	2.34	0.52
1:Y:40:ASP:C	1:Y:42:ASP:N	2.56	0.52
1:Y:50:THR:C	1:Y:52:GLN:H	2.18	0.51
1:Y:28:TYR:O	1:Y:73:PHE:CE1	2.63	0.51
1:Y:276:PHE:O	1:Y:279:ALA:HB3	2.10	0.51
1:Y:31:GLY:HA2	1:Y:34:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:19:LEU:O	1:Y:22:LEU:N	2.44	0.51
1:Y:1:MET:HB2	2:E:33:ALA:CB	2.41	0.51
1:Y:61:LEU:HD11	1:Y:192:ILE:HG23	1.93	0.51
1:Y:78:MET:O	1:Y:80:TYR:N	2.39	0.51
1:Y:274:ILE:HD11	1:Y:375:LEU:HD13	1.92	0.50
1:Y:64:GLY:C	1:Y:66:ASN:H	2.17	0.50
1:Y:190:ALA:HB2	2:E:41:PHE:HE1	1.75	0.50
1:Y:411:THR:C	1:Y:413:ARG:H	2.18	0.50
1:Y:45:GLN:HG2	1:Y:69:ARG:HA	1.93	0.50
1:Y:289:ALA:N	1:Y:290:PRO:HD3	2.27	0.50
1:Y:347:ILE:HB	1:Y:350:ILE:HB	1.92	0.50
1:Y:161:GLN:O	1:Y:165:ILE:HG22	2.11	0.50
1:Y:206:LEU:C	1:Y:208:ARG:N	2.68	0.50
1:Y:35:PRO:HA	1:Y:41:LEU:HD13	1.94	0.50
1:Y:59:ILE:HD11	1:Y:75:LEU:HA	1.94	0.50
1:Y:304:PHE:CD1	1:Y:314:ILE:HG21	2.47	0.50
1:Y:396:PHE:C	1:Y:398:GLY:H	2.20	0.50
1:Y:39:VAL:CG1	1:Y:44:ILE:HB	2.43	0.49
1:Y:170:TRP:HE1	1:Y:174:ARG:HE	1.60	0.49
2:E:48:TYR:HB3	2:E:52:PHE:CZ	2.47	0.49
1:Y:383:GLN:HA	1:Y:386:GLN:HB2	1.94	0.49
2:E:31:THR:HA	2:E:34:ILE:HD12	1.95	0.49
1:Y:326:TYR:C	1:Y:328:ALA:H	2.19	0.49
1:Y:44:ILE:HA	1:Y:142:PHE:HD2	1.78	0.49
1:Y:1:MET:C	2:E:33:ALA:HB2	2.38	0.49
1:Y:38:GLY:O	1:Y:144:LEU:HG	2.12	0.48
1:Y:193:VAL:HG23	2:E:45:LEU:CD1	2.43	0.48
1:Y:39:VAL:HG11	1:Y:44:ILE:HB	1.95	0.48
1:Y:59:ILE:HG12	1:Y:67:PHE:CD1	2.48	0.48
1:Y:238:GLU:HG2	2:E:20:THR:O	2.13	0.48
1:Y:36:THR:HB	1:Y:39:VAL:HB	1.94	0.48
1:Y:98:GLU:HA	1:Y:101:SER:HB3	1.96	0.48
1:Y:206:LEU:O	1:Y:211:GLU:N	2.46	0.48
1:Y:342:GLU:HG3	1:Y:342:GLU:O	2.12	0.48
2:E:40:ALA:O	2:E:44:ILE:HD12	2.14	0.48
1:Y:14:LEU:HD21	1:Y:415:VAL:HG13	1.94	0.48
1:Y:307:THR:HG21	1:Y:394:ILE:HA	1.96	0.48
1:Y:73:PHE:CZ	1:Y:168:LEU:HD13	2.48	0.48
1:Y:184:THR:O	1:Y:186:LEU:HB3	2.13	0.48
1:Y:383:GLN:O	1:Y:387:ASN:N	2.47	0.48
1:Y:57:GLY:HA2	1:Y:394:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:29:ARG:O	1:Y:32:ALA:HB3	2.13	0.48
1:Y:156:VAL:O	1:Y:160:THR:OG1	2.30	0.48
1:Y:190:ALA:HB1	2:E:45:LEU:HD21	1.94	0.48
1:Y:40:ASP:C	1:Y:43:LYS:H	2.11	0.47
1:Y:47:PHE:O	1:Y:53:GLY:HA3	2.14	0.47
1:Y:111:ILE:O	1:Y:115:THR:OG1	2.25	0.47
1:Y:266:LEU:HA	1:Y:367:LEU:HD22	1.95	0.47
1:Y:228:PHE:CB	2:E:31:THR:HG23	2.45	0.47
1:Y:47:PHE:HD1	1:Y:141:ARG:NH2	2.13	0.47
2:E:45:LEU:HA	2:E:48:TYR:CD1	2.50	0.47
2:E:51:VAL:C	2:E:53:ARG:H	2.22	0.47
1:Y:24:VAL:O	1:Y:28:TYR:N	2.47	0.47
1:Y:212:VAL:HG21	1:Y:390:GLY:HA3	1.95	0.47
1:Y:304:PHE:CE1	1:Y:314:ILE:HD13	2.51	0.46
1:Y:130:LEU:HG	1:Y:134:PHE:HD1	1.80	0.46
1:Y:47:PHE:CE2	1:Y:134:PHE:CE2	3.03	0.46
1:Y:212:VAL:HG22	1:Y:216:ALA:HB3	1.95	0.46
1:Y:33:PHE:HE1	2:E:49:ASP:OD2	1.98	0.46
1:Y:44:ILE:HG13	1:Y:48:LEU:HD11	1.98	0.46
1:Y:196:TRP:CD1	1:Y:395:ALA:HB1	2.49	0.46
1:Y:318:LEU:O	1:Y:322:PHE:HB2	2.15	0.46
1:Y:48:LEU:HD21	1:Y:134:PHE:CE1	2.51	0.46
1:Y:76:GLY:C	1:Y:168:LEU:HD23	2.41	0.46
1:Y:43:LYS:O	1:Y:142:PHE:HA	2.16	0.46
1:Y:340:LEU:HD22	1:Y:345:GLY:HA3	1.98	0.46
2:E:16:LEU:HA	2:E:19:VAL:CG2	2.44	0.45
1:Y:36:THR:C	1:Y:38:GLY:H	2.23	0.45
2:E:39:LEU:O	2:E:39:LEU:HG	2.17	0.45
1:Y:33:PHE:CE1	2:E:49:ASP:OD2	2.70	0.45
1:Y:183:GLY:O	1:Y:184:THR:O	2.34	0.45
1:Y:410:ASP:HA	1:Y:413:ARG:HB3	1.99	0.45
1:Y:27:ALA:O	1:Y:30:LEU:HB3	2.17	0.45
1:Y:34:ILE:HA	1:Y:35:PRO:HD2	1.82	0.45
1:Y:175:ILE:HG22	1:Y:180:ILE:O	2.17	0.45
1:Y:235:GLN:HG3	1:Y:409:LEU:HD21	1.99	0.45
1:Y:238:GLU:O	2:E:19:VAL:HG13	2.17	0.45
1:Y:50:THR:O	1:Y:54:GLY:CA	2.64	0.45
1:Y:5:PHE:HB2	1:Y:412:LEU:HD22	1.98	0.44
1:Y:50:THR:OG1	1:Y:53:GLY:N	2.48	0.44
1:Y:79:PRO:O	1:Y:119:GLY:HA2	2.17	0.44
1:Y:228:PHE:HB3	2:E:31:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:324:TYR:HA	1:Y:368:THR:HG21	1.99	0.44
1:Y:28:TYR:HA	1:Y:171:MET:HE1	1.98	0.44
1:Y:272:ILE:N	1:Y:273:PRO:HD2	2.31	0.44
1:Y:326:TYR:HA	1:Y:329:VAL:HG22	2.00	0.44
1:Y:377:LEU:HG	1:Y:381:LEU:HD11	1.98	0.44
1:Y:176:THR:HA	1:Y:181:GLY:O	2.16	0.44
1:Y:307:THR:O	1:Y:383:GLN:NE2	2.50	0.44
1:Y:212:VAL:HG22	1:Y:213:ASN:OD1	2.18	0.44
2:E:17:ALA:C	2:E:19:VAL:N	2.74	0.44
1:Y:116:ARG:O	1:Y:120:ILE:HG13	2.18	0.43
1:Y:1:MET:H3	1:Y:1:MET:HG3	1.48	0.43
1:Y:289:ALA:N	1:Y:290:PRO:CD	2.80	0.43
1:Y:46:GLU:HA	1:Y:49:ARG:HG3	2.00	0.43
1:Y:312:LEU:O	1:Y:316:VAL:HG23	2.18	0.43
1:Y:39:VAL:C	1:Y:41:LEU:N	2.77	0.43
1:Y:281:LEU:HD13	1:Y:318:LEU:HD23	1.99	0.43
1:Y:383:GLN:NE2	1:Y:392:HIS:HE1	2.01	0.43
1:Y:326:TYR:CD1	1:Y:329:VAL:HG21	2.53	0.43
1:Y:43:LYS:HB3	1:Y:142:PHE:HA	2.01	0.43
1:Y:101:SER:HB2	1:Y:111:ILE:HD12	2.01	0.43
1:Y:304:PHE:O	1:Y:305:ASN:C	2.62	0.43
1:Y:22:LEU:HD23	1:Y:25:LEU:HD12	2.01	0.42
1:Y:55:VAL:C	1:Y:57:GLY:N	2.74	0.42
1:Y:237:ALA:O	1:Y:265:LYS:HD3	2.19	0.42
1:Y:382:PRO:O	1:Y:386:GLN:N	2.50	0.42
1:Y:407:VAL:O	1:Y:411:THR:OG1	2.29	0.42
1:Y:183:GLY:C	1:Y:184:THR:O	2.59	0.42
1:Y:288:ALA:HA	1:Y:297:LEU:HD22	2.00	0.42
1:Y:34:ILE:HB	1:Y:72:ILE:HG12	2.01	0.42
1:Y:1:MET:H3	2:E:30:GLY:HA2	1.84	0.42
1:Y:49:ARG:NE	1:Y:68:GLU:CD	2.77	0.42
1:Y:212:VAL:C	1:Y:213:ASN:ND2	2.78	0.42
1:Y:367:LEU:C	1:Y:369:LEU:H	2.28	0.42
1:Y:48:LEU:HA	1:Y:53:GLY:HA3	2.02	0.42
1:Y:239:ARG:CB	2:E:19:VAL:HG22	2.49	0.42
1:Y:17:ARG:HD3	1:Y:180:ILE:HA	2.01	0.42
1:Y:43:LYS:O	1:Y:142:PHE:CD2	2.73	0.42
1:Y:270:GLY:O	1:Y:274:ILE:HG12	2.20	0.42
1:Y:375:LEU:CA	1:Y:378:VAL:HB	2.49	0.42
1:Y:238:GLU:OE2	1:Y:265:LYS:NZ	2.53	0.42
1:Y:56:PHE:O	1:Y:59:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:325:VAL:HA	1:Y:328:ALA:HB3	2.02	0.41
1:Y:354:GLU:O	1:Y:357:VAL:HB	2.20	0.41
1:Y:11:ILE:HA	1:Y:12:PRO:HD3	1.86	0.41
1:Y:206:LEU:HB3	1:Y:211:GLU:HB3	1.86	0.41
1:Y:386:GLN:OE1	1:Y:392:HIS:HA	2.20	0.41
1:Y:47:PHE:CD1	1:Y:141:ARG:NH2	2.88	0.41
2:E:42:MET:HA	2:E:45:LEU:HD12	2.02	0.41
1:Y:4:ALA:O	1:Y:8:ALA:N	2.53	0.41
1:Y:206:LEU:C	1:Y:208:ARG:H	2.28	0.41
1:Y:274:ILE:CD1	1:Y:319:VAL:HG13	2.44	0.41
2:E:17:ALA:C	2:E:19:VAL:H	2.28	0.41
1:Y:1:MET:N	2:E:29:GLU:O	2.52	0.41
1:Y:205:GLY:HA2	1:Y:208:ARG:HH11	1.85	0.41
1:Y:196:TRP:CZ2	1:Y:401:LEU:HB2	2.56	0.41
1:Y:273:PRO:HB3	1:Y:323:THR:HA	2.01	0.41
1:Y:386:GLN:HB3	1:Y:392:HIS:ND1	2.36	0.41
1:Y:396:PHE:C	1:Y:398:GLY:N	2.79	0.40
1:Y:148:SER:C	1:Y:150:GLY:N	2.79	0.40
1:Y:1:MET:H1	2:E:29:GLU:CD	2.30	0.40
1:Y:352:PRO:HA	1:Y:356:THR:OG1	2.21	0.40
1:Y:237:ALA:O	1:Y:238:GLU:HB3	2.22	0.40
1:Y:239:ARG:CD	2:E:19:VAL:HG22	2.49	0.40
2:E:28:VAL:HG12	2:E:32:GLN:CD	2.45	0.40
1:Y:193:VAL:CG1	1:Y:404:VAL:HG22	2.50	0.40
1:Y:239:ARG:HD2	2:E:19:VAL:CG2	2.50	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:42:ASP:CB	1:Y:208:ARG:O[5_455]	1.56	0.64
1:Y:42:ASP:CA	1:Y:208:ARG:O[5_455]	1.66	0.54
1:Y:42:ASP:CG	1:Y:208:ARG:O[5_455]	2.04	0.16

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	Y	411/434 (95%)	335 (82%)	56 (14%)	20 (5%)	1	15
2	E	44/60 (73%)	31 (70%)	11 (25%)	2 (4%)	2	16
All	All	455/494 (92%)	366 (80%)	67 (15%)	22 (5%)	2	16

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	40	ASP
1	Y	45	GLN
1	Y	46	GLU
1	Y	184	THR
1	Y	185	SER
1	Y	309	PRO
1	Y	181	GLY
1	Y	197	LEU
1	Y	212	VAL
1	Y	371	GLY
1	Y	35	PRO
1	Y	37	PRO
1	Y	394	ILE
2	E	17	ALA
1	Y	51	ALA
1	Y	402	LEU
2	E	27	VAL
1	Y	12	PRO
1	Y	79	PRO
1	Y	96	ALA
1	Y	405	VAL
1	Y	38	GLY

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	Y	332/347 (96%)	288 (87%)	44 (13%)	4	14
2	E	38/51 (74%)	32 (84%)	6 (16%)	2	12
All	All	370/398 (93%)	320 (86%)	50 (14%)	4	14

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	1	MET
1	Y	14	LEU
1	Y	21	THR
1	Y	28	TYR
1	Y	30	LEU
1	Y	59	ILE
1	Y	77	ILE
1	Y	91	VAL
1	Y	110	ILE
1	Y	156	VAL
1	Y	162	VAL
1	Y	165	ILE
1	Y	180	ILE
1	Y	185	SER
1	Y	188	ILE
1	Y	192	ILE
1	Y	194	VAL
1	Y	201	LEU
1	Y	208	ARG
1	Y	209	THR
1	Y	212	VAL
1	Y	213	ASN
1	Y	217	PHE
1	Y	238	GLU
1	Y	258	GLN
1	Y	262	ILE
1	Y	271	VAL
1	Y	272	ILE
1	Y	294	ASN
1	Y	314	ILE
1	Y	319	VAL
1	Y	340	LEU
1	Y	341	ARG
1	Y	342	GLU
1	Y	368	THR

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Mol	Chain	Res	Type
1	Y	373	LEU
1	Y	378	VAL
1	Y	379	THR
1	Y	391	ILE
1	Y	394	ILE
1	Y	402	LEU
1	Y	407	VAL
1	Y	409	LEU
1	Y	414	GLN
2	E	15	GLU
2	E	21	TRP
2	E	25	GLU
2	E	28	VAL
2	E	34	ILE
2	E	44	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	88	GLN
1	Y	161	GLN
1	Y	182	ASN
1	Y	267	ASN
1	Y	282	GLN
1	Y	294	ASN
1	Y	387	ASN
1	Y	392	HIS
1	Y	414	GLN
2	E	32	GLN

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 [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	Y	415/434 (95%)	0.74	60 (14%) 6 14	325, 368, 371, 373	1 (0%)
2	E	46/60 (76%)	0.35	3 (6%) 25 29	364, 368, 371, 372	0
All	All	461/494 (93%)	0.70	63 (13%) 6 15	325, 368, 371, 373	1 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	263	PRO	10.4
1	Y	83	ALA	8.0
1	Y	114	TYR	6.5
1	Y	262	ILE	6.4
1	Y	225	VAL	6.2
1	Y	145	PRO	6.2
1	Y	222	ALA	6.2
1	Y	77	ILE	5.7
1	Y	78	MET	5.4
1	Y	82	THR	4.6
1	Y	294	ASN	4.5
1	Y	264	ILE	4.4
1	Y	223	PHE	4.1
1	Y	219	PHE	3.8
1	Y	393	SER	3.6
1	Y	110	ILE	3.6
1	Y	304	PHE	3.6
1	Y	295	PRO	3.4
1	Y	241	ILE	3.3
2	E	20	THR	3.3
1	Y	308	ARG	3.2
1	Y	202	ARG	3.1
1	Y	80	TYR	3.1
1	Y	293	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	Y	303	PHE	3.0
1	Y	199	GLN	3.0
1	Y	158	VAL	3.0
1	Y	20	PHE	2.9
1	Y	170	TRP	2.8
1	Y	62	PHE	2.8
2	E	26	GLN	2.8
1	Y	261	TYR	2.7
1	Y	381	LEU	2.7
1	Y	221	LEU	2.6
1	Y	292	GLN	2.6
1	Y	115	THR	2.6
1	Y	332	ASP	2.6
1	Y	81	ILE	2.5
1	Y	360	LEU	2.5
1	Y	342	GLU	2.4
1	Y	116	ARG	2.4
1	Y	268	ALA	2.4
1	Y	392	HIS	2.4
1	Y	299	GLY	2.3
1	Y	260	THR	2.3
1	Y	12	PRO	2.3
1	Y	302	ASN	2.2
1	Y	159	VAL	2.2
1	Y	130	LEU	2.2
1	Y	144	LEU	2.2
1	Y	227	ALA	2.2
1	Y	285	ILE	2.2
1	Y	270	GLY	2.2
1	Y	149	PRO	2.2
1	Y	188	ILE	2.2
1	Y	300	ILE	2.2
1	Y	296	VAL	2.1
1	Y	154	TRP	2.1
1	Y	23	LEU	2.1
1	Y	336	ILE	2.1
2	E	56	ILE	2.1
1	Y	369	LEU	2.1
1	Y	358	LYS	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.