



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:48 PM UTC

PDB ID : 2ZJS / pdb_00002zjs
Title : Crystal Structure of SecYE translocon from *Thermus thermophilus* with a Fab fragment
Authors : Tsukazaki, T.; Mori, H.; Fukai, S.; Ishitani, R.; Perederina, A.; Vassylyev, D.G.; Ito, K.; Nureki, O.
Deposited on : 2008-03-08
Resolution : 3.20 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

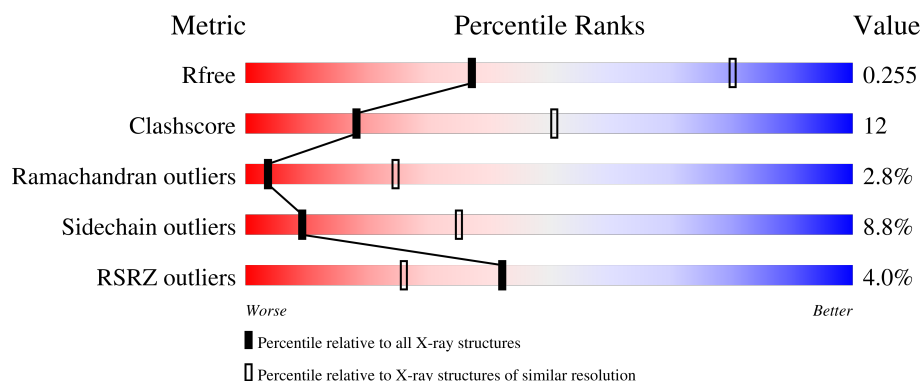
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

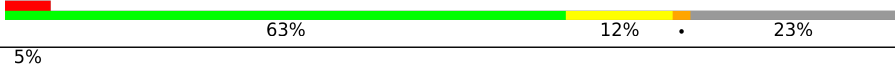
The reported resolution of this entry is 3.20 Å.

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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	
2	E	60	
3	H	221	
4	L	214	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6932 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
			3227	2155	529	537	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
			369	245	61	62	1			

- Molecule 3 is a protein called Fab56 (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	220	Total	C	N	O	S	0	0	0
			1667	1059	270	331	7			

- Molecule 4 is a protein called Fab56 (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	214	Total	C	N	O	S	0	0	0
			1667	1032	282	346	7			

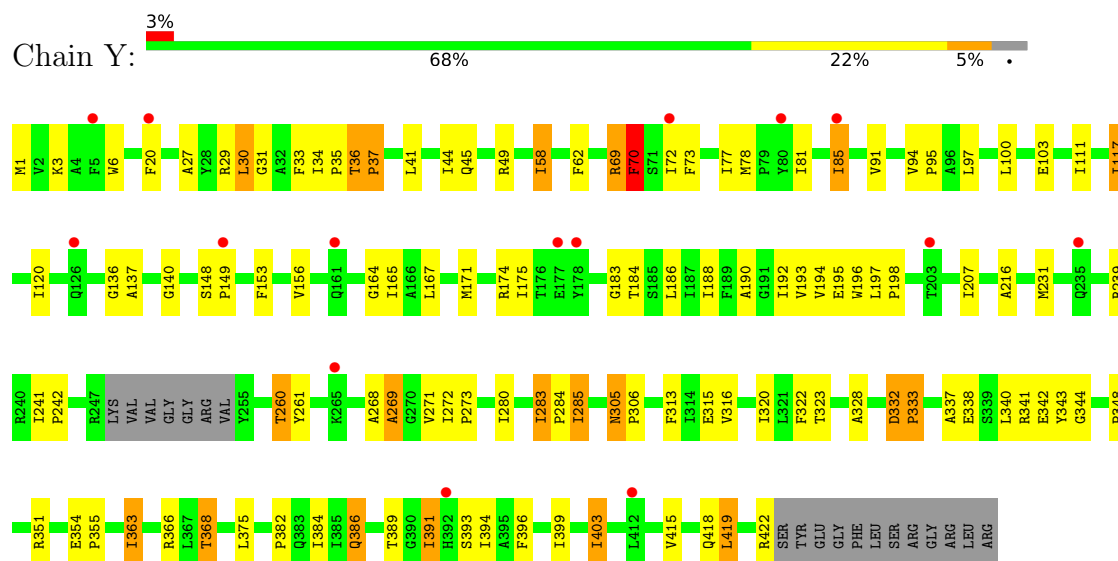
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Y	1	Total 1	Zn 1	0	0
5	L	1	Total 1	Zn 1	0	0

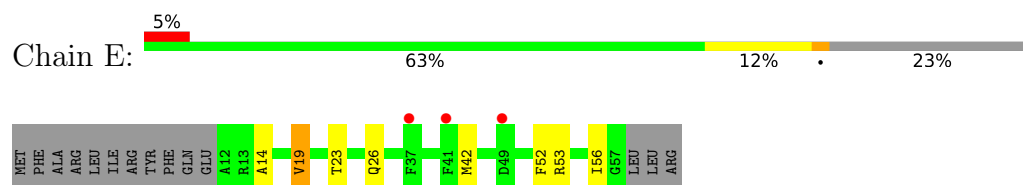
3 Residue-property plots [i](#)

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.

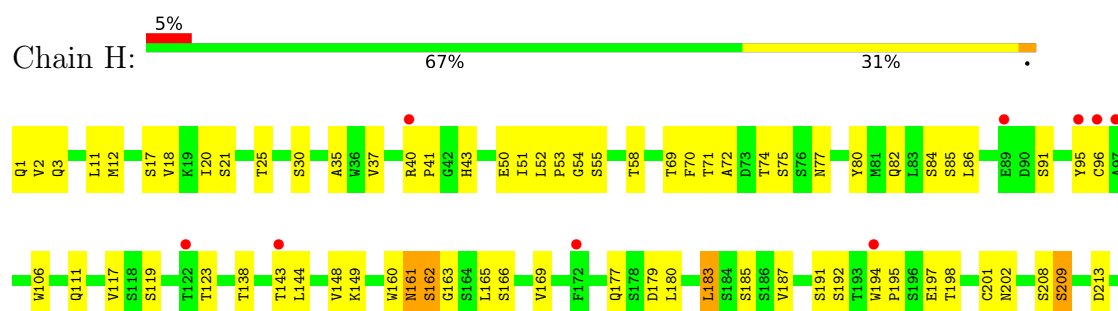
• Molecule 1: Preprotein translocase SecY subunit



• Molecule 2: Preprotein translocase SecE subunit

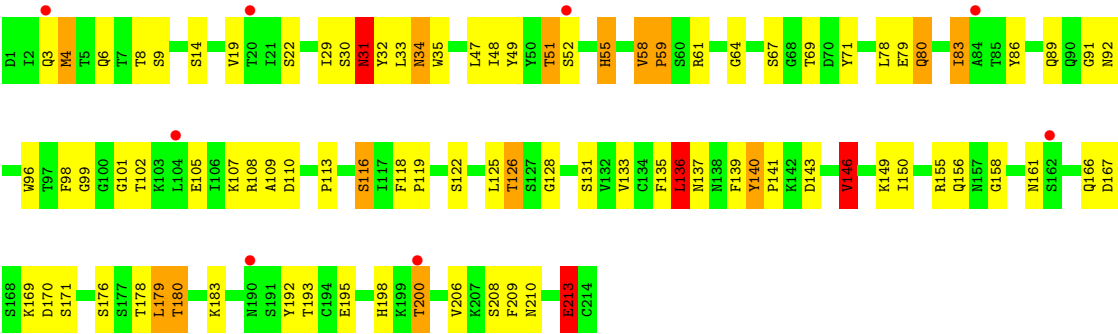


• Molecule 3: Fab56 (heavy chain)





● Molecule 4: Fab56 (light chain)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.10Å 103.07Å 78.00Å 90.00° 105.18° 90.00°	Depositor
Resolution (Å)	48.43 – 3.20 48.43 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.43-3.20) 94.0 (48.43-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2, REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.280 0.257 , 0.255	Depositor DCC
R_{free} test set	1102 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	104.2	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 92.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6932	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.54	3/3306 (0.1%)	0.94	7/4500 (0.2%)
2	E	0.46	0/376	0.84	0/511
3	H	0.49	0/1716	0.83	1/2350 (0.0%)
4	L	0.52	0/1702	0.91	4/2310 (0.2%)
All	All	0.52	3/7100 (0.0%)	0.90	12/9671 (0.1%)

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
4	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	283	ILE	CA-CB	5.91	1.57	1.54
1	Y	103	GLU	C-N	5.32	1.41	1.33
1	Y	103	GLU	C-O	5.06	1.31	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	137	ASN	N-CA-C	8.40	124.14	112.04
1	Y	36	THR	CA-C-N	7.74	129.51	119.84
1	Y	36	THR	C-N-CA	7.74	129.51	119.84
1	Y	148	SER	CA-C-N	6.37	127.80	119.84
1	Y	148	SER	C-N-CA	6.37	127.80	119.84
3	H	43	HIS	N-CA-C	5.96	118.10	108.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3	GLN	N-CA-C	5.56	117.72	108.99
1	Y	137	ALA	N-CA-C	5.24	117.42	111.02
1	Y	305	ASN	CA-C-N	5.18	124.85	119.56
1	Y	305	ASN	C-N-CA	5.18	124.85	119.56
4	L	31	ASN	N-CA-C	5.09	121.65	110.80
4	L	146	VAL	CB-CA-C	-5.05	106.03	111.59

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	136	LEU	Peptide

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	3227	0	3373	70	0
2	E	369	0	384	6	0
3	H	1667	0	1608	35	0
4	L	1667	0	1589	65	0
5	L	1	0	0	0	0
5	Y	1	0	0	0	0
All	All	6932	0	6954	168	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 12.

All (168) 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:332:ASP:HB2	1:Y:333:PRO:HD3	1.24	1.15
3:H:12:MET:HE3	3:H:18:VAL:HG22	1.33	1.05
1:Y:332:ASP:CB	1:Y:333:PRO:HD3	2.03	0.88
4:L:141:PRO:HD2	4:L:198:HIS:HE1	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:52:SER:HB2	4:L:64:GLY:HA3	1.58	0.84
1:Y:192:ILE:HD13	1:Y:403:ILE:HD11	1.59	0.84
1:Y:332:ASP:HB2	1:Y:333:PRO:CD	2.09	0.78
4:L:141:PRO:HD2	4:L:198:HIS:CE1	2.20	0.77
3:H:106:TRP:HH2	4:L:96:TRP:CD1	2.02	0.76
4:L:136:LEU:HD11	4:L:146:VAL:HG13	1.65	0.76
1:Y:190:ALA:O	1:Y:194:VAL:HG23	1.86	0.75
1:Y:45:GLN:HB3	1:Y:49:ARG:HH21	1.51	0.75
1:Y:33:PHE:O	1:Y:35:PRO:HD3	1.89	0.72
4:L:4:MET:HE1	4:L:29:ILE:HD11	1.72	0.72
1:Y:394:ILE:H	1:Y:394:ILE:HD12	1.54	0.72
4:L:167:ASP:HB3	4:L:170:ASP:O	1.91	0.70
3:H:71:THR:HB	3:H:80:TYR:HB2	1.72	0.70
4:L:108:ARG:HH12	4:L:170:ASP:HB2	1.59	0.67
3:H:37:VAL:HB	3:H:95:TYR:HB2	1.77	0.67
4:L:61:ARG:HH12	4:L:79:GLU:HB2	1.61	0.66
3:H:18:VAL:HG23	3:H:86:LEU:HD11	1.79	0.64
4:L:80:GLN:HE21	4:L:83:ILE:HG21	1.63	0.64
1:Y:175:ILE:HB	1:Y:183:GLY:HA2	1.80	0.63
3:H:161:ASN:C	3:H:163:GLY:H	2.05	0.63
4:L:195:GLU:HG2	4:L:206:VAL:HG22	1.79	0.63
4:L:55:HIS:HB3	4:L:58:VAL:HG12	1.81	0.62
4:L:140:TYR:O	4:L:141:PRO:C	2.42	0.62
4:L:198:HIS:ND1	4:L:200:THR:HB	2.14	0.62
1:Y:167:LEU:O	1:Y:171:MET:HG3	2.00	0.61
4:L:34:ASN:ND2	4:L:49:TYR:O	2.33	0.61
4:L:19:VAL:HG21	4:L:78:LEU:HD12	1.83	0.61
4:L:31:ASN:HB3	4:L:51:THR:OG1	2.00	0.60
4:L:6:GLN:HE21	4:L:99:GLY:HA3	1.66	0.60
4:L:198:HIS:HB3	4:L:200:THR:HG22	1.84	0.59
1:Y:272:ILE:N	1:Y:273:PRO:HD2	2.17	0.59
1:Y:29:ARG:CZ	1:Y:194:VAL:HG11	2.32	0.59
4:L:122:SER:HA	4:L:125:LEU:HD12	1.85	0.58
1:Y:338:GLU:O	1:Y:341:ARG:HB2	2.04	0.58
4:L:19:VAL:HG21	4:L:78:LEU:CD1	2.33	0.58
4:L:133:VAL:HG13	4:L:178:THR:HG22	1.86	0.57
4:L:80:GLN:O	4:L:83:ILE:HG22	2.04	0.57
4:L:48:ILE:HG21	4:L:52:SER:C	2.29	0.57
1:Y:366:ARG:HH11	2:E:14:ALA:HB3	1.70	0.57
2:E:52:PHE:O	2:E:56:ILE:HG13	2.05	0.56
1:Y:81:ILE:O	1:Y:85:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:313:PHE:HA	1:Y:316:VAL:HG12	1.88	0.56
1:Y:332:ASP:CB	1:Y:333:PRO:CD	2.74	0.55
3:H:106:TRP:HH2	4:L:96:TRP:CG	2.25	0.55
4:L:105:GLU:HG3	4:L:166:GLN:NE2	2.22	0.54
1:Y:316:VAL:O	1:Y:320:ILE:HG12	2.07	0.54
4:L:91:GLY:C	4:L:96:TRP:HZ3	2.16	0.54
1:Y:77:ILE:HG12	1:Y:184:THR:HG23	1.89	0.54
4:L:118:PHE:CE1	4:L:135:PHE:HD1	2.27	0.53
3:H:160:TRP:O	3:H:162:SER:N	2.42	0.53
3:H:30:SER:HA	3:H:53:PRO:HB2	1.90	0.53
3:H:91:SER:HB3	3:H:117:VAL:H	1.74	0.53
3:H:106:TRP:CH2	4:L:96:TRP:CD1	2.92	0.53
4:L:47:LEU:HD11	4:L:86:TYR:HE2	1.73	0.53
1:Y:260:THR:HG22	1:Y:261:TYR:H	1.73	0.53
1:Y:58:ILE:HD11	1:Y:285:ILE:HD13	1.90	0.52
1:Y:136:GLY:HA2	1:Y:140:GLY:HA2	1.92	0.52
1:Y:241:ILE:HD11	1:Y:363:ILE:HG21	1.92	0.52
4:L:89:GLN:HB2	4:L:98:PHE:CD2	2.44	0.52
1:Y:216:ALA:HB1	1:Y:389:THR:HG23	1.93	0.51
1:Y:69:ARG:O	1:Y:70:PHE:C	2.53	0.51
4:L:193:THR:HA	4:L:208:SER:HB3	1.92	0.51
3:H:194:TRP:O	3:H:195:PRO:C	2.53	0.51
3:H:1:GLN:HG2	3:H:2:VAL:H	1.76	0.50
1:Y:192:ILE:HD13	1:Y:403:ILE:CD1	2.36	0.50
4:L:58:VAL:HG22	4:L:59:PRO:HD2	1.92	0.50
4:L:136:LEU:HD11	4:L:146:VAL:CG1	2.38	0.50
4:L:150:ILE:CD1	4:L:155:ARG:HD3	2.42	0.50
1:Y:394:ILE:HD12	1:Y:394:ILE:N	2.25	0.50
1:Y:20:PHE:HZ	1:Y:174:ARG:HB3	1.78	0.49
4:L:118:PHE:HE1	4:L:135:PHE:HD1	1.59	0.49
3:H:149:LYS:HE2	3:H:177:GLN:OE1	2.12	0.49
1:Y:354:GLU:HB3	1:Y:355:PRO:HD3	1.94	0.49
1:Y:418:GLN:HE21	1:Y:422:ARG:HE	1.61	0.49
1:Y:386:GLN:HG2	1:Y:391:ILE:O	2.13	0.49
1:Y:389:THR:HG22	1:Y:391:ILE:H	1.78	0.49
1:Y:415:VAL:O	1:Y:419:LEU:HB2	2.13	0.49
3:H:53:PRO:HA	3:H:72:ALA:CB	2.43	0.49
1:Y:72:ILE:O	1:Y:164:GLY:HA3	2.13	0.48
1:Y:328:ALA:HB2	1:Y:368:THR:HG21	1.95	0.48
3:H:161:ASN:C	3:H:163:GLY:N	2.70	0.48
3:H:165:LEU:HD13	3:H:187:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:149:LYS:HB2	4:L:193:THR:HB	1.96	0.48
1:Y:306:PRO:HB3	1:Y:315:GLU:OE1	2.14	0.48
3:H:53:PRO:HA	3:H:72:ALA:HB1	1.96	0.47
3:H:148:VAL:HB	3:H:183:LEU:HB3	1.96	0.47
1:Y:193:VAL:O	1:Y:196:TRP:HB2	2.14	0.47
4:L:110:ASP:HA	4:L:140:TYR:HB3	1.96	0.47
1:Y:337:ALA:HA	1:Y:340:LEU:HD12	1.97	0.47
1:Y:382:PRO:O	1:Y:386:GLN:HB2	2.14	0.47
1:Y:100:LEU:HB2	1:Y:111:ILE:HD11	1.97	0.47
3:H:70:PHE:HA	3:H:80:TYR:O	2.15	0.47
3:H:18:VAL:O	3:H:82:GLN:HA	2.15	0.47
4:L:108:ARG:HG2	4:L:109:ALA:N	2.30	0.47
1:Y:3:LYS:HA	1:Y:6:TRP:HB2	1.97	0.47
4:L:67:SER:HA	4:L:71:TYR:CE2	2.50	0.47
4:L:213:GLU:HG2	4:L:213:GLU:O	2.15	0.46
4:L:192:TYR:O	4:L:208:SER:HB2	2.15	0.46
1:Y:94:VAL:HA	1:Y:95:PRO:HD3	1.82	0.46
1:Y:268:ALA:O	1:Y:269:ALA:C	2.59	0.46
1:Y:41:LEU:HD22	1:Y:69:ARG:HA	1.98	0.46
1:Y:197:LEU:HA	2:E:42:MET:HE3	1.97	0.46
1:Y:41:LEU:HD13	1:Y:69:ARG:HB2	1.99	0.45
3:H:160:TRP:HA	3:H:201:CYS:HA	1.97	0.45
4:L:135:PHE:C	4:L:136:LEU:HD23	2.42	0.45
1:Y:323:THR:HG21	1:Y:375:LEU:HD12	1.99	0.45
1:Y:20:PHE:CZ	1:Y:174:ARG:HB3	2.51	0.45
1:Y:394:ILE:H	1:Y:394:ILE:CD1	2.27	0.45
1:Y:27:ALA:HA	1:Y:30:LEU:HB3	1.99	0.44
2:E:23:THR:HB	2:E:26:GLN:HB3	1.98	0.44
4:L:150:ILE:HD12	4:L:155:ARG:HD3	1.99	0.44
4:L:29:ILE:HG23	4:L:92:ASN:HB2	1.98	0.44
1:Y:94:VAL:HB	1:Y:97:LEU:HD12	1.99	0.44
1:Y:97:LEU:HA	1:Y:100:LEU:HD12	1.98	0.44
1:Y:231:MET:HE2	1:Y:231:MET:HB3	1.90	0.44
4:L:33:LEU:HD13	4:L:71:TYR:CD1	2.53	0.44
1:Y:351:ARG:NH1	3:H:50:GLU:OE2	2.51	0.43
3:H:208:SER:O	3:H:209:SER:C	2.60	0.43
3:H:12:MET:CE	3:H:18:VAL:HG22	2.24	0.43
4:L:118:PHE:CE1	4:L:135:PHE:CD1	3.06	0.43
1:Y:36:THR:HA	1:Y:37:PRO:HD2	1.80	0.43
3:H:202:ASN:OD1	3:H:213:ASP:HB3	2.17	0.43
4:L:116:SER:HB2	4:L:118:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:119:PRO:HB3	4:L:209:PHE:CE1	2.54	0.43
3:H:160:TRP:HZ3	3:H:216:ILE:HD11	1.83	0.43
4:L:158:GLY:O	4:L:179:LEU:HA	2.19	0.43
3:H:51:ILE:HG13	3:H:58:THR:HG22	2.00	0.43
1:Y:117:ILE:HA	1:Y:120:ILE:HG22	2.01	0.42
4:L:107:LYS:HA	4:L:107:LYS:HD2	1.92	0.42
2:E:53:ARG:HH11	2:E:56:ILE:HD11	1.83	0.42
4:L:35:TRP:CD1	4:L:52:SER:HB3	2.53	0.42
4:L:86:TYR:O	4:L:101:GLY:HA2	2.20	0.42
4:L:166:GLN:NE2	4:L:171:SER:HB2	2.35	0.42
1:Y:305:ASN:HA	1:Y:306:PRO:HD3	1.83	0.42
1:Y:280:ILE:HG13	1:Y:322:PHE:CZ	2.55	0.41
4:L:30:SER:O	4:L:32:TYR:CD1	2.73	0.41
4:L:210:ASN:HB2	4:L:213:GLU:HB3	2.02	0.41
1:Y:283:ILE:HB	1:Y:284:PRO:HD3	2.01	0.41
1:Y:167:LEU:HD22	1:Y:171:MET:SD	2.60	0.41
1:Y:62:PHE:CD2	1:Y:78:MET:HE3	2.55	0.41
1:Y:174:ARG:HA	1:Y:174:ARG:HD3	1.81	0.41
1:Y:272:ILE:N	1:Y:273:PRO:CD	2.82	0.41
4:L:113:PRO:HG3	4:L:139:PHE:HB3	2.02	0.41
1:Y:188:ILE:HG22	1:Y:403:ILE:HD13	2.02	0.41
4:L:9:SER:O	4:L:102:THR:HA	2.20	0.41
4:L:155:ARG:HG3	4:L:156:GLN:N	2.35	0.41
1:Y:153:PHE:HA	1:Y:156:VAL:HG12	2.01	0.41
1:Y:239:ARG:HB2	2:E:19:VAL:HG22	2.03	0.41
3:H:166:SER:O	3:H:169:VAL:HG22	2.21	0.41
3:H:179:ASP:OD1	3:H:180:LEU:HG	2.21	0.41
4:L:140:TYR:HB3	4:L:141:PRO:HD3	2.02	0.41
3:H:149:LYS:HE3	4:L:180:THR:HG21	2.02	0.41
4:L:83:ILE:HG23	4:L:83:ILE:O	2.21	0.41
1:Y:31:GLY:HA2	1:Y:34:ILE:HG12	2.03	0.40
3:H:35:ALA:O	3:H:96:CYS:HA	2.21	0.40
3:H:144:LEU:HB3	3:H:216:ILE:HD13	2.03	0.40
4:L:118:PHE:HA	4:L:119:PRO:HD3	1.85	0.40
4:L:126:THR:C	4:L:128:GLY:H	2.29	0.40
1:Y:393:SER:OG	1:Y:396:PHE:HD1	2.04	0.40
3:H:52:LEU:O	3:H:55:SER:O	2.38	0.40
3:H:191:SER:O	3:H:195:PRO:HD2	2.21	0.40
4:L:125:LEU:HB3	4:L:183:LYS:HE3	2.04	0.40
1:Y:242:PRO:O	1:Y:348:PRO:HD2	2.21	0.40
1:Y:197:LEU:HB3	1:Y:198:PRO:HD3	2.03	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	Y	411/434 (95%)	373 (91%)	29 (7%)	9 (2%)	5	29
2	E	44/60 (73%)	39 (89%)	5 (11%)	0	100	100
3	H	218/221 (99%)	190 (87%)	19 (9%)	9 (4%)	2	17
4	L	212/214 (99%)	195 (92%)	10 (5%)	7 (3%)	3	21
All	All	885/929 (95%)	797 (90%)	63 (7%)	25 (3%)	4	25

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	70	PHE
1	Y	269	ALA
1	Y	332	ASP
3	H	162	SER
4	L	213	GLU
1	Y	344	GLY
1	Y	368	THR
3	H	54	GLY
3	H	85	SER
3	H	161	ASN
3	H	209	SER
4	L	31	ASN
4	L	83	ILE
4	L	169	LYS
1	Y	149	PRO
3	H	41	PRO
3	H	75	SER
4	L	140	TYR
1	Y	37	PRO
1	Y	342	GLU

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Mol	Chain	Res	Type
3	H	84	SER
4	L	51	THR
3	H	77	ASN
1	Y	333	PRO
4	L	59	PRO

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%)	307 (92%)	25 (8%)	12	42
2	E	38/51 (74%)	37 (97%)	1 (3%)	40	69
3	H	187/188 (100%)	168 (90%)	19 (10%)	7	29
4	L	192/192 (100%)	171 (89%)	21 (11%)	6	26
All	All	749/778 (96%)	683 (91%)	66 (9%)	9	35

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	1	MET
1	Y	30	LEU
1	Y	44	ILE
1	Y	58	ILE
1	Y	69	ARG
1	Y	70	PHE
1	Y	73	PHE
1	Y	85	ILE
1	Y	91	VAL
1	Y	117	ILE
1	Y	165	ILE
1	Y	186	LEU
1	Y	195	GLU
1	Y	207	ILE
1	Y	260	THR
1	Y	271	VAL

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Mol	Chain	Res	Type
1	Y	285	ILE
1	Y	343	TYR
1	Y	363	ILE
1	Y	384	ILE
1	Y	386	GLN
1	Y	391	ILE
1	Y	399	ILE
1	Y	403	ILE
1	Y	419	LEU
2	E	19	VAL
3	H	3	GLN
3	H	11	LEU
3	H	17	SER
3	H	20	ILE
3	H	21	SER
3	H	25	THR
3	H	40	ARG
3	H	69	THR
3	H	74	THR
3	H	111	GLN
3	H	119	SER
3	H	123	THR
3	H	138	THR
3	H	143	THR
3	H	183	LEU
3	H	185	SER
3	H	192	SER
3	H	197	GLU
3	H	198	THR
4	L	4	MET
4	L	8	THR
4	L	14	SER
4	L	22	SER
4	L	34	ASN
4	L	55	HIS
4	L	58	VAL
4	L	69	THR
4	L	80	GLN
4	L	116	SER
4	L	126	THR
4	L	131	SER
4	L	136	LEU

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Mol	Chain	Res	Type
4	L	143	ASP
4	L	146	VAL
4	L	161	ASN
4	L	176	SER
4	L	179	LEU
4	L	180	THR
4	L	200	THR
4	L	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	52	GLN
1	Y	199	GLN
1	Y	302	ASN
1	Y	392	HIS
1	Y	418	GLN
3	H	39	GLN
3	H	105	ASN
3	H	161	ASN
4	L	6	GLN
4	L	38	GLN
4	L	77	ASN
4	L	80	GLN
4	L	190	ASN
4	L	210	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	Y	415/434 (95%)	0.23	15 (3%) 46 28	105, 127, 156, 163	0
2	E	46/60 (76%)	0.68	3 (6%) 25 16	133, 149, 163, 164	0
3	H	220/221 (99%)	0.35	10 (4%) 38 24	112, 125, 136, 145	0
4	L	214/214 (100%)	0.23	8 (3%) 45 28	104, 120, 128, 139	0
All	All	895/929 (96%)	0.28	36 (4%) 42 26	104, 124, 155, 164	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	37	PHE	5.8
1	Y	265	LYS	5.1
4	L	3	GLN	4.8
1	Y	178	TYR	4.5
4	L	84	ALA	4.0
1	Y	235	GLN	3.9
4	L	190	ASN	3.9
3	H	97	ALA	3.6
1	Y	203	THR	3.3
4	L	52	SER	3.3
2	E	41	PHE	3.0
1	Y	72	ILE	3.0
1	Y	20	PHE	2.9
1	Y	85	ILE	2.9
1	Y	80	TYR	2.9
1	Y	412	LEU	2.8
3	H	96	CYS	2.8
3	H	172	PHE	2.7
4	L	200	THR	2.7
4	L	20	THR	2.7
1	Y	5	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	Y	177	GLU	2.6
1	Y	149	PRO	2.6
1	Y	161	GLN	2.6
3	H	194	TRP	2.5
4	L	104	LEU	2.5
3	H	122	THR	2.4
1	Y	392	HIS	2.3
3	H	95	TYR	2.3
4	L	162	SER	2.3
1	Y	126	GLN	2.2
2	E	49	ASP	2.2
3	H	89	GLU	2.2
3	H	143	THR	2.1
3	H	40	ARG	2.1
3	H	217	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	Y	435	1/1	0.99	0.06	89,89,89,89	1
5	ZN	L	223	1/1	0.99	0.04	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.