



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:30 AM UTC

PDB ID : 4IL3 / pdb_00004il3
Title : Crystal Structure of S. mikatae Ste24p
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Deposited on : 2012-12-28
Resolution : 3.10 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

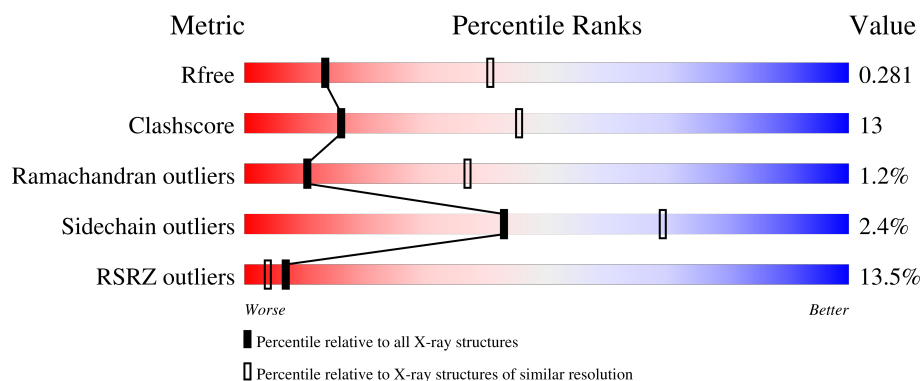
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	461	
1	B	461	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6975 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 Ste24p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3445	2281	537	612	15			
1	B	431	Total	C	N	O	S	0	0	0
			3528	2343	548	622	15			

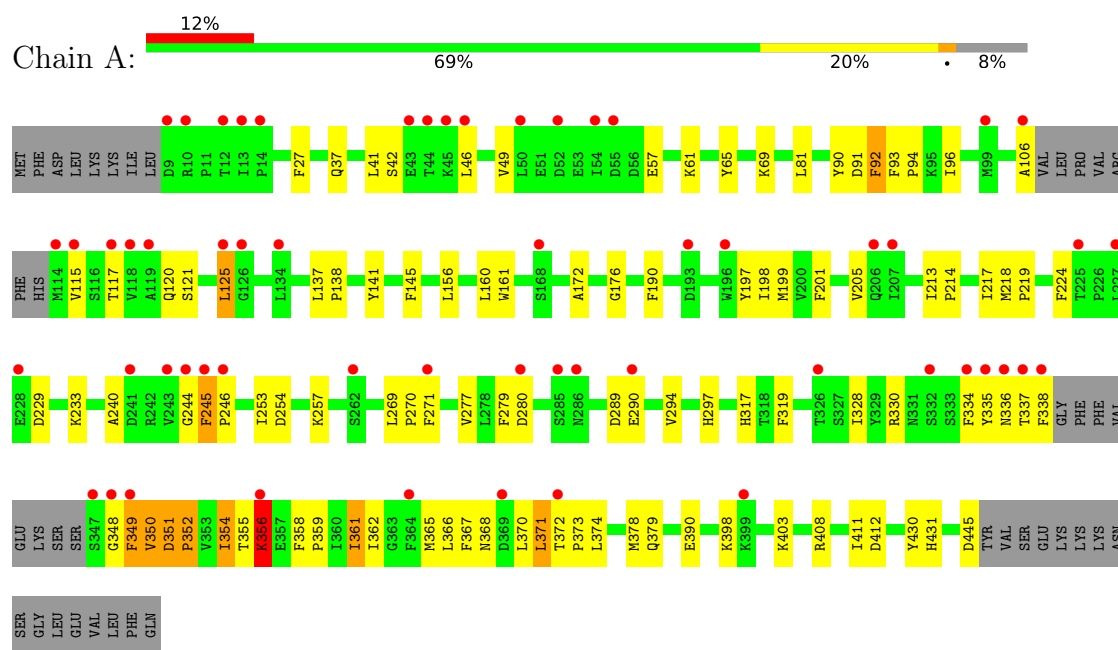
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

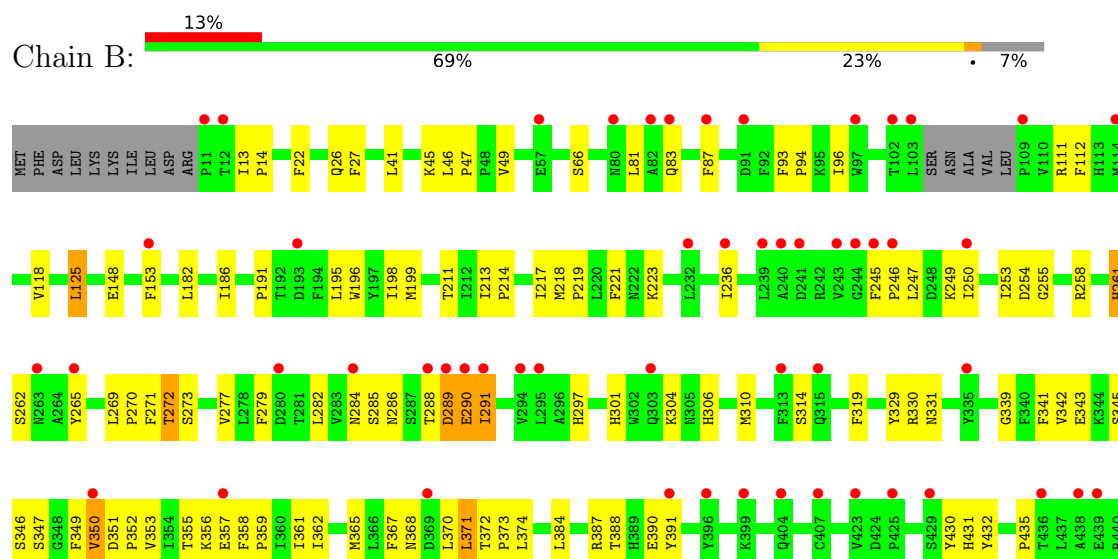
3 Residue-property plots

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: Ste24p



• Molecule 1: Ste24p



L441	T442	A443	L444	D445	Y446	VAL	SER	GLU	LYS	LYS	ASN	SER	GLY	LEU	GLU	VAL	LEU	PHE	GLN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	143.53Å 143.53Å 197.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.10 48.45 – 3.10	Depositor EDS
% Data completeness (in resolution range)	60.0 (48.45-3.10) 52.4 (48.45-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.270 , 0.293 0.282 , 0.281	Depositor DCC
R_{free} test set	1349 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6975	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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	A	0.34	1/3539 (0.0%)	0.75	7/4799 (0.1%)
1	B	0.35	2/3629 (0.1%)	0.71	4/4920 (0.1%)
All	All	0.34	3/7168 (0.0%)	0.73	11/9719 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	HIS	ND1-CE1	5.30	1.37	1.32
1	B	301	HIS	ND1-CE1	5.27	1.37	1.32
1	A	431	HIS	ND1-CE1	5.10	1.37	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	B	261	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	A	431	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	A	351	ASP	N-CA-C	6.42	118.01	110.31
1	A	269	LEU	CA-C-N	-6.22	113.27	119.99
1	A	269	LEU	C-N-CA	-6.22	113.27	119.99
1	B	301	HIS	CB-CG-ND1	5.73	131.29	122.70
1	A	431	HIS	CB-CG-ND1	5.69	131.23	122.70
1	B	261	HIS	CB-CG-ND1	5.59	131.09	122.70
1	A	336	ASN	N-CA-C	5.51	118.47	111.69
1	A	290	GLU	N-CA-C	-5.10	106.89	113.01

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	3445	0	3472	90	0
1	B	3528	0	3555	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	6975	0	7027	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 13.

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)
1:B:288:THR:O	1:B:290:GLU:N	1.99	0.95
1:A:351:ASP:HB2	1:A:352:PRO:HD2	1.63	0.77
1:A:297:HIS:CE1	1:A:390:GLU:OE1	2.40	0.74
1:B:346:SER:O	1:B:347:SER:OG	2.04	0.74
1:A:335:TYR:CD1	1:A:354:ILE:HD13	2.25	0.70
1:A:245:PHE:N	1:A:246:PRO:CD	2.55	0.69
1:B:297:HIS:CE1	1:B:390:GLU:OE1	2.46	0.69
1:A:335:TYR:CG	1:A:354:ILE:HD13	2.29	0.68
1:A:94:PRO:HB3	1:A:354:ILE:HD11	1.76	0.68
1:B:288:THR:C	1:B:290:GLU:N	2.53	0.64
1:A:350:VAL:HG12	1:A:351:ASP:OD1	1.98	0.64
1:A:351:ASP:O	1:A:352:PRO:C	2.41	0.63
1:A:351:ASP:OD1	1:A:351:ASP:N	2.32	0.62
1:A:337:THR:HA	1:A:355:THR:HA	1.81	0.62
1:A:354:ILE:HD12	1:A:354:ILE:N	2.15	0.62
1:A:337:THR:OG1	1:A:358:PHE:CD1	2.53	0.61
1:A:348:GLY:C	1:A:349:PHE:CG	2.80	0.60
1:B:199:MET:HE1	1:B:319:PHE:HA	1.84	0.60
1:A:351:ASP:HB2	1:A:352:PRO:CD	2.32	0.60
1:A:125:LEU:HG	1:A:361:ILE:HD11	1.84	0.59
1:A:317:HIS:ND1	1:A:378:MET:SD	2.76	0.58
1:A:348:GLY:O	1:A:349:PHE:CB	2.51	0.58
1:A:337:THR:OG1	1:A:337:THR:O	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASN:HA	1:B:371:LEU:HD12	1.86	0.57
1:B:351:ASP:OD1	1:B:351:ASP:N	2.38	0.57
1:A:335:TYR:OH	1:A:362:ILE:HG13	2.05	0.56
1:B:153:PHE:CE2	1:B:261:HIS:CE1	2.93	0.56
1:A:213:ILE:CG1	1:A:214:PRO:HD3	2.34	0.56
1:A:213:ILE:HG12	1:A:214:PRO:HD3	1.88	0.56
1:B:41:LEU:HD11	1:B:66:SER:HB3	1.88	0.55
1:B:349:PHE:CD2	1:B:350:VAL:HG12	2.42	0.55
1:B:356:LYS:O	1:B:357:GLU:C	2.49	0.55
1:B:291:ILE:O	1:B:291:ILE:HG22	2.06	0.55
1:A:348:GLY:O	1:A:349:PHE:CG	2.60	0.54
1:A:351:ASP:CB	1:A:352:PRO:HD2	2.36	0.54
1:A:190:PHE:CE1	1:A:197:TYR:CZ	2.96	0.54
1:A:348:GLY:C	1:A:349:PHE:CD1	2.85	0.54
1:B:289:ASP:O	1:B:290:GLU:CG	2.55	0.54
1:B:358:PHE:HB3	1:B:359:PRO:CD	2.39	0.53
1:B:148:GLU:OE1	1:B:153:PHE:CE1	2.62	0.53
1:A:337:THR:HB	1:A:356:LYS:O	2.09	0.53
1:B:289:ASP:O	1:B:290:GLU:HG3	2.08	0.53
1:B:371:LEU:C	1:B:373:PRO:HD2	2.34	0.53
1:A:224:PHE:CD1	1:A:253:ILE:HG22	2.44	0.53
1:B:371:LEU:O	1:B:374:LEU:N	2.42	0.53
1:B:93:PHE:HB2	1:B:94:PRO:HD3	1.91	0.52
1:B:350:VAL:O	1:B:350:VAL:HG13	2.09	0.52
1:B:153:PHE:HE2	1:B:261:HIS:CE1	2.27	0.52
1:B:282:LEU:O	1:B:285:SER:O	2.27	0.52
1:A:371:LEU:C	1:A:373:PRO:HD2	2.35	0.52
1:A:348:GLY:O	1:A:349:PHE:HB2	2.09	0.52
1:B:430:TYR:CD2	1:B:431:HIS:CD2	2.97	0.52
1:A:244:GLY:C	1:A:246:PRO:HD2	2.34	0.52
1:B:118:VAL:O	1:B:118:VAL:HG12	2.10	0.52
1:A:368:ASN:HA	1:A:371:LEU:HD12	1.92	0.51
1:B:341:PHE:CD2	1:B:345:SER:HB2	2.44	0.51
1:B:223:LYS:N	1:B:254:ASP:OD1	2.42	0.51
1:B:357:GLU:OE1	1:B:357:GLU:N	2.44	0.51
1:B:270:PRO:O	1:B:271:PHE:HB2	2.10	0.51
1:B:27:PHE:CG	1:B:81:LEU:HD22	2.46	0.50
1:A:41:LEU:HD12	1:A:42:SER:N	2.26	0.50
1:A:245:PHE:N	1:A:246:PRO:HD3	2.25	0.50
1:A:372:THR:CG2	1:A:373:PRO:HD3	2.42	0.50
1:B:191:PRO:O	1:B:329:TYR:OH	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:TYR:CE1	1:B:435:PRO:CG	2.95	0.50
1:A:106:ALA:HB3	1:A:115:VAL:HG22	1.94	0.50
1:B:211:THR:HG23	1:B:269:LEU:O	2.12	0.50
1:B:13:ILE:HG23	1:B:14:PRO:HD2	1.93	0.49
1:B:349:PHE:CE2	1:B:350:VAL:HG12	2.48	0.49
1:B:83:GLN:O	1:B:87:PHE:HB2	2.12	0.49
1:A:57:GLU:OE2	1:A:61:LYS:HE2	2.12	0.49
1:B:289:ASP:C	1:B:290:GLU:HG3	2.38	0.49
1:A:371:LEU:O	1:A:374:LEU:N	2.46	0.49
1:B:384:LEU:HA	1:B:387:ARG:NH1	2.28	0.49
1:B:342:VAL:HG12	1:B:357:GLU:O	2.13	0.48
1:A:93:PHE:N	1:A:94:PRO:CD	2.77	0.48
1:A:372:THR:HG23	1:A:373:PRO:HD3	1.96	0.48
1:B:262:SER:HB3	1:B:282:LEU:HD13	1.94	0.48
1:B:342:VAL:CG1	1:B:357:GLU:O	2.62	0.48
1:A:367:PHE:CZ	1:A:371:LEU:HD21	2.48	0.47
1:A:253:ILE:HG23	1:A:277:VAL:HG13	1.96	0.47
1:B:346:SER:O	1:B:347:SER:CB	2.62	0.47
1:B:358:PHE:CD1	1:B:358:PHE:N	2.82	0.47
1:A:408:ARG:NH2	1:A:412:ASP:OD1	2.47	0.47
1:B:245:PHE:CD1	1:B:246:PRO:O	2.67	0.47
1:A:445:ASP:OD1	1:A:445:ASP:C	2.56	0.47
1:A:337:THR:O	1:A:338:PHE:HB3	2.14	0.47
1:B:372:THR:CG2	1:B:373:PRO:HD3	2.45	0.47
1:A:49:VAL:HG22	1:A:49:VAL:O	2.15	0.47
1:A:349:PHE:O	1:A:350:VAL:HG22	2.15	0.47
1:A:253:ILE:HD11	1:A:279:PHE:CE1	2.51	0.46
1:A:335:TYR:CD2	1:A:354:ILE:HB	2.50	0.46
1:A:224:PHE:CE1	1:A:253:ILE:HG22	2.50	0.46
1:B:387:ARG:NH2	1:B:432:TYR:O	2.49	0.46
1:A:65:TYR:CE2	1:A:69:LYS:HD2	2.51	0.46
1:A:254:ASP:HA	1:A:280:ASP:HB2	1.98	0.46
1:B:247:LEU:HD23	1:B:249:LYS:N	2.31	0.46
1:A:361:ILE:HD11	1:A:365:MET:HE3	1.97	0.46
1:A:46:LEU:O	1:A:46:LEU:HD12	2.16	0.46
1:B:339:GLY:O	1:B:352:PRO:HD2	2.16	0.45
1:A:334:PHE:CE1	1:A:366:LEU:HD22	2.51	0.45
1:A:361:ILE:CG1	1:A:365:MET:HE3	2.47	0.45
1:B:45:LYS:O	1:B:45:LYS:HG2	2.16	0.45
1:B:195:LEU:HD23	1:B:196:TRP:CZ3	2.51	0.45
1:B:269:LEU:HG	1:B:272:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:PHE:CD1	1:A:349:PHE:N	2.82	0.45
1:B:269:LEU:N	1:B:270:PRO:HA	2.32	0.45
1:B:286:ASN:O	1:B:291:ILE:HD11	2.16	0.45
1:A:137:LEU:HB3	1:A:138:PRO:HD3	1.99	0.45
1:A:240:ALA:O	1:A:244:GLY:O	2.34	0.45
1:B:330:ARG:O	1:B:331:ASN:C	2.58	0.45
1:A:365:MET:O	1:A:368:ASN:HB3	2.17	0.45
1:B:371:LEU:O	1:B:372:THR:C	2.60	0.45
1:A:190:PHE:CD1	1:A:197:TYR:CE2	3.05	0.44
1:A:328:ILE:HG22	1:A:328:ILE:O	2.16	0.44
1:A:218:MET:N	1:A:219:PRO:CD	2.80	0.44
1:B:342:VAL:C	1:B:343:GLU:HG2	2.41	0.44
1:B:350:VAL:O	1:B:350:VAL:CG1	2.65	0.44
1:A:199:MET:HE1	1:A:319:PHE:HA	1.99	0.44
1:B:372:THR:HG23	1:B:373:PRO:HD3	1.98	0.44
1:A:330:ARG:O	1:A:358:PHE:CE2	2.70	0.44
1:A:371:LEU:O	1:A:372:THR:C	2.61	0.44
1:B:272:THR:HG22	1:B:273:SER:H	1.83	0.44
1:B:353:VAL:HG23	1:B:353:VAL:O	2.16	0.44
1:A:160:LEU:HD21	1:A:257:LYS:HD2	2.00	0.44
1:B:253:ILE:HG12	1:B:254:ASP:N	2.30	0.44
1:A:372:THR:CG2	1:A:373:PRO:CD	2.96	0.44
1:B:388:THR:HA	1:B:391:TYR:CD2	2.53	0.44
1:A:213:ILE:N	1:A:214:PRO:CD	2.82	0.43
1:B:341:PHE:CD1	1:B:351:ASP:OD2	2.72	0.43
1:A:270:PRO:HA	1:A:271:PHE:HA	1.66	0.43
1:B:27:PHE:CD1	1:B:27:PHE:C	2.97	0.43
1:B:213:ILE:HB	1:B:214:PRO:HD3	2.01	0.43
1:B:22:PHE:HB3	1:B:372:THR:CG2	2.48	0.43
1:B:365:MET:O	1:B:368:ASN:HB3	2.18	0.43
1:B:374:LEU:C	1:B:374:LEU:HD23	2.44	0.43
1:B:46:LEU:HA	1:B:47:PRO:HD3	1.91	0.43
1:A:398:LYS:CG	1:A:403:LYS:HB2	2.48	0.43
1:A:92:PHE:O	1:A:96:ILE:HG13	2.18	0.43
1:B:218:MET:N	1:B:219:PRO:CD	2.82	0.43
1:B:269:LEU:C	1:B:269:LEU:HD13	2.43	0.43
1:B:289:ASP:O	1:B:290:GLU:CB	2.67	0.43
1:B:372:THR:N	1:B:373:PRO:HD2	2.34	0.43
1:B:391:TYR:CE1	1:B:435:PRO:HG2	2.54	0.43
1:B:444:LEU:O	1:B:445:ASP:HB2	2.19	0.43
1:A:355:THR:O	1:A:356:LYS:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLY:HA3	1:B:279:PHE:CE2	2.53	0.42
1:B:125:LEU:HG	1:B:361:ILE:HD11	2.02	0.42
1:A:141:TYR:HB2	1:A:161:TRP:CH2	2.54	0.42
1:A:379:GLN:HG2	1:A:430:TYR:CE1	2.54	0.42
1:B:41:LEU:C	1:B:41:LEU:HD23	2.45	0.42
1:B:236:ILE:HD12	1:B:250:ILE:HG12	2.00	0.42
1:A:90:TYR:O	1:A:91:ASP:C	2.63	0.42
1:A:145:PHE:CZ	1:A:156:LEU:CD1	3.02	0.42
1:B:182:LEU:O	1:B:186:ILE:HG12	2.19	0.42
1:B:372:THR:CG2	1:B:373:PRO:CD	2.98	0.42
1:A:294:VAL:O	1:A:297:HIS:HB3	2.19	0.42
1:B:153:PHE:CD1	1:B:153:PHE:C	2.97	0.42
1:A:37:GLN:HA	1:A:37:GLN:OE1	2.19	0.42
1:A:117:THR:O	1:A:120:GLN:NE2	2.53	0.42
1:B:198:ILE:HD12	1:B:198:ILE:C	2.45	0.42
1:B:211:THR:OG1	1:B:270:PRO:HD3	2.20	0.42
1:B:304:LYS:HB2	1:B:306:HIS:CD2	2.54	0.42
1:A:125:LEU:HD12	1:A:361:ILE:HD12	2.02	0.41
1:A:229:ASP:HA	1:A:233:LYS:HD3	2.02	0.41
1:B:221:PHE:O	1:B:258:ARG:NH2	2.53	0.41
1:B:349:PHE:O	1:B:350:VAL:C	2.63	0.41
1:A:27:PHE:CD1	1:A:27:PHE:C	2.98	0.41
1:A:198:ILE:C	1:A:198:ILE:HD12	2.45	0.41
1:B:26:GLN:OE1	1:B:26:GLN:HA	2.20	0.41
1:B:153:PHE:CZ	1:B:261:HIS:CE1	3.07	0.41
1:B:444:LEU:O	1:B:445:ASP:CB	2.68	0.41
1:B:359:PRO:HG2	1:B:362:ILE:HG13	2.02	0.41
1:A:156:LEU:HD12	1:A:156:LEU:O	2.21	0.41
1:A:172:ALA:O	1:A:176:GLY:HA3	2.21	0.41
1:B:265:TYR:HB2	1:B:277:VAL:CG1	2.51	0.41
1:B:367:PHE:CZ	1:B:371:LEU:HD21	2.56	0.41
1:A:121:SER:HB3	1:A:361:ILE:HG21	2.03	0.41
1:A:372:THR:N	1:A:373:PRO:HD2	2.35	0.41
1:B:111:ARG:O	1:B:112:PHE:C	2.64	0.41
1:A:93:PHE:HB2	1:A:94:PRO:HD3	2.03	0.41
1:B:49:VAL:HG12	1:B:49:VAL:O	2.21	0.41
1:A:201:PHE:O	1:A:205:VAL:HG23	2.21	0.40
1:A:27:PHE:CG	1:A:81:LEU:HD22	2.56	0.40
1:B:355:THR:OG1	1:B:356:LYS:N	2.52	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	416/461 (90%)	378 (91%)	33 (8%)	5 (1%)	10	37
1	B	427/461 (93%)	388 (91%)	34 (8%)	5 (1%)	10	37
All	All	843/922 (91%)	766 (91%)	67 (8%)	10 (1%)	10	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	PHE
1	A	352	PRO
1	A	356	LYS
1	B	290	GLU
1	B	284	ASN
1	B	289	ASP
1	B	291	ILE
1	A	359	PRO
1	B	350	VAL
1	A	245	PHE

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	388/425 (91%)	377 (97%)	11 (3%)	38	66
1	B	397/425 (93%)	389 (98%)	8 (2%)	48	72
All	All	785/850 (92%)	766 (98%)	19 (2%)	43	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	PHE
1	A	125	LEU
1	A	217	ILE
1	A	289	ASP
1	A	350	VAL
1	A	354	ILE
1	A	356	LYS
1	A	361	ILE
1	A	370	LEU
1	A	371	LEU
1	A	411	ILE
1	B	96	ILE
1	B	125	LEU
1	B	217	ILE
1	B	272	THR
1	B	310	MET
1	B	314	SER
1	B	370	LEU
1	B	371	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	80	ASN
1	A	98	HIS
1	A	261	HIS
1	A	331	ASN
1	A	389	HIS
1	B	317	HIS
1	B	379	GLN
1	B	405	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/461 (91%)	0.63	57 (13%) 7 4	56, 85, 142, 194	0
1	B	431/461 (93%)	0.72	58 (13%) 7 4	51, 89, 146, 192	0
All	All	853/922 (92%)	0.68	115 (13%) 7 4	51, 86, 145, 194	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	GLN	7.0
1	A	245	PHE	6.6
1	B	289	ASP	6.4
1	A	338	PHE	5.8
1	A	246	PRO	5.4
1	B	244	GLY	5.4
1	B	243	VAL	5.3
1	A	356	LYS	4.8
1	A	44	THR	4.7
1	B	439	GLU	4.5
1	A	43	GLU	4.4
1	A	46	LEU	4.4
1	B	436	THR	4.2
1	B	250	ILE	4.1
1	A	271	PHE	4.1
1	B	245	PHE	4.0
1	B	396	TYR	4.0
1	B	291	ILE	3.9
1	B	241	ASP	3.9
1	A	334	PHE	3.9
1	B	153	PHE	3.8
1	B	444	LEU	3.8
1	B	425	PRO	3.8
1	A	241	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	265	TYR	3.8
1	A	12	THR	3.8
1	B	445	ASP	3.7
1	B	407	CYS	3.7
1	B	11	PRO	3.5
1	A	228	GLU	3.5
1	A	9	ASP	3.5
1	B	438	ALA	3.3
1	A	117	THR	3.3
1	A	45	LYS	3.2
1	B	240	ALA	3.2
1	A	280	ASP	3.2
1	B	335	TYR	3.2
1	A	244	GLY	3.1
1	A	196	TRP	3.1
1	A	115	VAL	3.1
1	A	119	ALA	3.1
1	A	134	LEU	3.1
1	A	106	ALA	3.1
1	B	423	VAL	3.1
1	B	97	TRP	3.0
1	B	399	LYS	3.0
1	B	295	LEU	3.0
1	A	118	VAL	3.0
1	A	364	PHE	3.0
1	A	349	PHE	2.9
1	A	99	MET	2.9
1	B	315	GLN	2.9
1	A	335	TYR	2.9
1	B	236	ILE	2.8
1	B	294	VAL	2.8
1	B	263	ASN	2.8
1	B	239	LEU	2.8
1	A	348	GLY	2.7
1	B	82	ALA	2.7
1	A	243	VAL	2.7
1	A	290	GLU	2.6
1	B	369	ASP	2.6
1	A	336	ASN	2.6
1	B	288	THR	2.6
1	A	285	SER	2.6
1	A	125	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	337	THR	2.6
1	A	114	MET	2.6
1	A	207	ILE	2.6
1	A	225	THR	2.6
1	B	350	VAL	2.5
1	B	429	SER	2.5
1	A	10	ARG	2.5
1	B	441	LEU	2.5
1	B	290	GLU	2.5
1	B	114	MET	2.4
1	B	12	THR	2.4
1	B	446	TYR	2.4
1	A	168	SER	2.4
1	B	57	GLU	2.4
1	A	52	ASP	2.4
1	B	193	ASP	2.4
1	B	103	LEU	2.4
1	A	55	ASP	2.3
1	A	227	LEU	2.3
1	A	332	SER	2.3
1	B	83	GLN	2.3
1	B	313	PHE	2.3
1	B	404	GLN	2.3
1	B	87	PHE	2.3
1	A	286	ASN	2.3
1	B	284	ASN	2.3
1	A	13	ILE	2.2
1	B	102	THR	2.2
1	A	50	LEU	2.2
1	A	326	THR	2.2
1	A	347	SER	2.2
1	B	232	LEU	2.2
1	A	369	ASP	2.2
1	B	442	THR	2.1
1	B	391	TYR	2.1
1	B	246	PRO	2.1
1	B	80	ASN	2.1
1	A	54	ILE	2.1
1	A	372	THR	2.1
1	B	109	PRO	2.1
1	A	193	ASP	2.1
1	B	280	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	303	GLN	2.1
1	B	357	GLU	2.1
1	A	262	SER	2.1
1	B	91	ASP	2.1
1	A	14	PRO	2.1
1	A	126	GLY	2.0
1	A	399	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](#)

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
2	ZN	A	501	1/1	0.93	0.05	74,74,74,74	0
2	ZN	B	501	1/1	0.95	0.06	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.