



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:29 PM UTC

PDB ID : 6N3I / pdb_00006n3i
Title : Crystal structure of a double Trp XylE mutants (G58W/L315W)
Authors : Jiang, X.; Wu, J.P.; Yan, N.
Deposited on : 2018-11-15
Resolution : 3.69 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

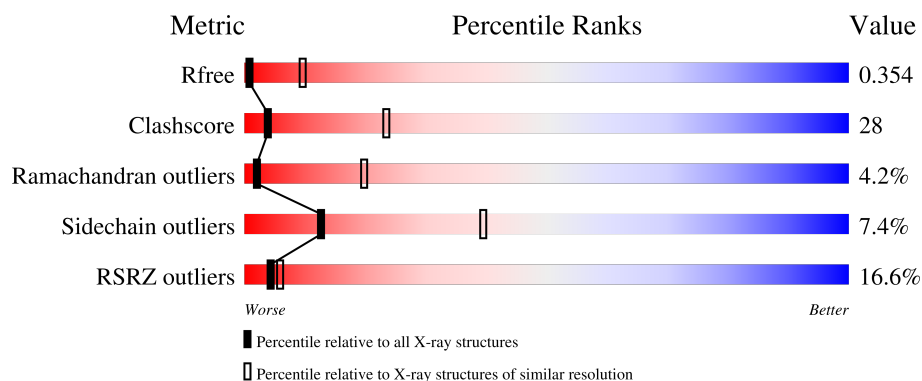
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.69 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	518	15% 45% 42% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3641 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 D-xylose transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3641	2411	579	627	24			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP C3SHS4
A	-25	GLY	-	expression tag	UNP C3SHS4
A	-24	SER	-	expression tag	UNP C3SHS4
A	-23	SER	-	expression tag	UNP C3SHS4
A	-22	HIS	-	expression tag	UNP C3SHS4
A	-21	HIS	-	expression tag	UNP C3SHS4
A	-20	HIS	-	expression tag	UNP C3SHS4
A	-19	HIS	-	expression tag	UNP C3SHS4
A	-18	HIS	-	expression tag	UNP C3SHS4
A	-17	HIS	-	expression tag	UNP C3SHS4
A	-16	SER	-	expression tag	UNP C3SHS4
A	-15	SER	-	expression tag	UNP C3SHS4
A	-14	GLY	-	expression tag	UNP C3SHS4
A	-13	LEU	-	expression tag	UNP C3SHS4
A	-12	VAL	-	expression tag	UNP C3SHS4
A	-11	PRO	-	expression tag	UNP C3SHS4
A	-10	ARG	-	expression tag	UNP C3SHS4
A	-9	GLY	-	expression tag	UNP C3SHS4
A	-8	SER	-	expression tag	UNP C3SHS4
A	-7	HIS	-	expression tag	UNP C3SHS4
A	-6	SER	-	expression tag	UNP C3SHS4
A	-5	ASP	-	expression tag	UNP C3SHS4
A	-4	GLU	-	expression tag	UNP C3SHS4
A	-3	VAL	-	expression tag	UNP C3SHS4
A	-2	ASP	-	expression tag	UNP C3SHS4
A	-1	ALA	-	expression tag	UNP C3SHS4
A	0	HIS	-	expression tag	UNP C3SHS4

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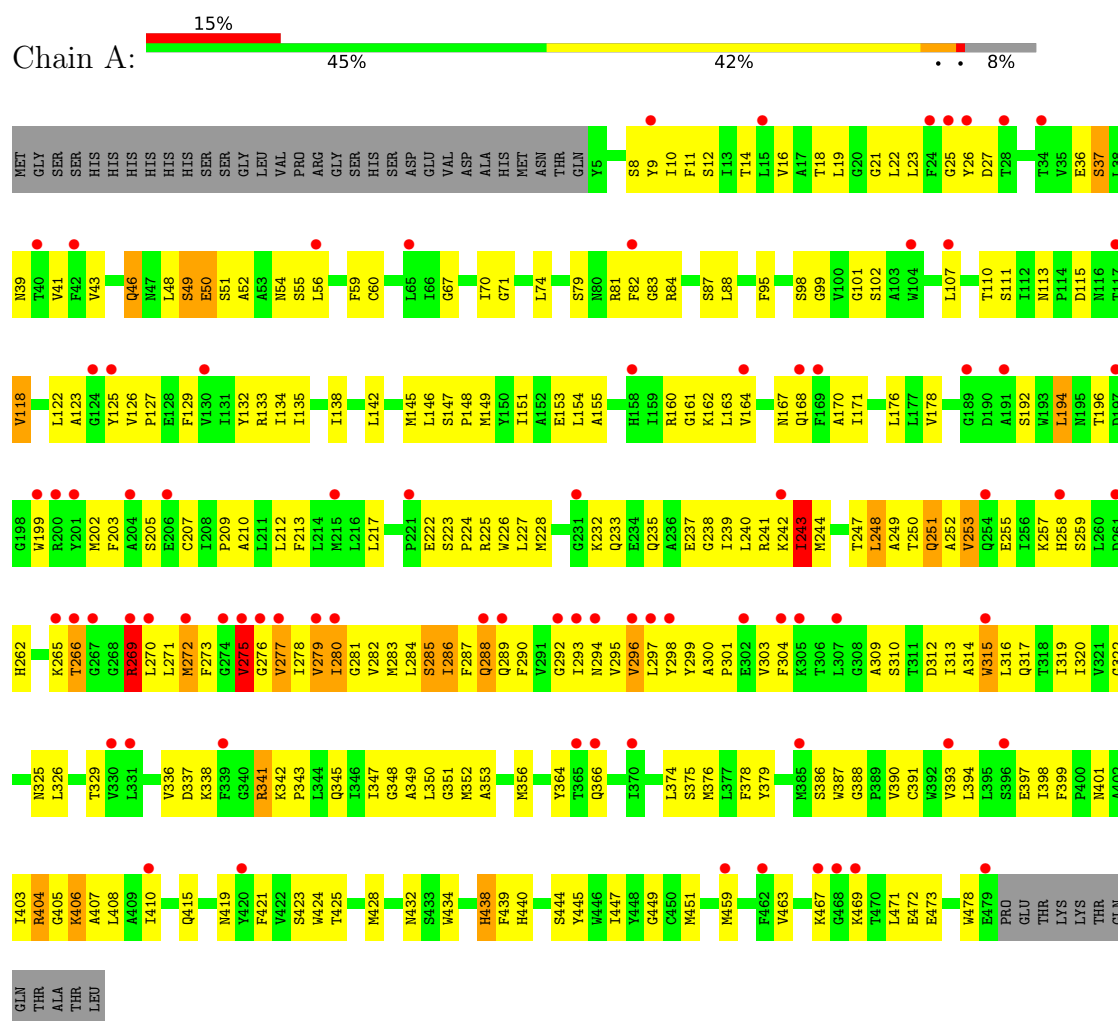
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Chain	Residue	Modelled	Actual	Comment	Reference
A	58	TRP	GLY	engineered mutation	UNP C3SHS4
A	315	TRP	LEU	engineered mutation	UNP C3SHS4

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: D-xylose transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.08Å 95.48Å 106.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.60 – 3.69 35.60 – 3.69	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.60-3.69) 98.9 (35.60-3.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.291 , 0.330 0.304 , 0.354	Depositor DCC
R_{free} test set	493 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	119.5	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3641	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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

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	0.42	0/3740	0.92	3/5096 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	GLN	N-CA-C	-7.82	104.22	114.31
1	A	251	GLN	CA-CB-CG	5.15	124.39	114.10
1	A	46	GLN	N-CA-C	-5.12	106.86	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	3641	0	3666	208	0
All	All	3641	0	3666	208	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 28.

All (208) 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:A:294:ASN:HB3	1:A:298:TYR:CE2	1.84	1.11
1:A:294:ASN:HB3	1:A:298:TYR:HE2	1.06	1.07
1:A:9:TYR:HD2	1:A:243:ILE:HG12	1.20	1.05
1:A:9:TYR:CD2	1:A:243:ILE:HG12	1.94	1.02
1:A:102:SER:HG	1:A:203:PHE:HD1	1.17	0.93
1:A:102:SER:OG	1:A:203:PHE:CD1	2.20	0.93
1:A:276:GLY:O	1:A:280:ILE:HG13	1.70	0.92
1:A:293:ILE:O	1:A:296:VAL:HG23	1.74	0.87
1:A:269:ARG:NH1	1:A:410:ILE:HD11	1.90	0.86
1:A:248:LEU:HD23	1:A:251:GLN:OE1	1.78	0.84
1:A:266:THR:HB	1:A:271:LEU:CD1	2.11	0.81
1:A:288:GLN:HE22	1:A:415:GLN:NE2	1.80	0.80
1:A:248:LEU:CD2	1:A:251:GLN:CD	2.55	0.79
1:A:294:ASN:O	1:A:298:TYR:CD2	2.35	0.79
1:A:300:ALA:N	1:A:301:PRO:HD2	1.97	0.79
1:A:146:LEU:HA	1:A:149:MET:HB3	1.66	0.77
1:A:269:ARG:HH21	1:A:269:ARG:HA	1.48	0.77
1:A:403:ILE:HA	1:A:406:LYS:HE3	1.68	0.76
1:A:248:LEU:CD2	1:A:251:GLN:OE1	2.32	0.76
1:A:289:GLN:NE2	1:A:294:ASN:HD21	1.83	0.76
1:A:294:ASN:O	1:A:298:TYR:HD2	1.69	0.75
1:A:9:TYR:CD2	1:A:243:ILE:CG1	2.69	0.73
1:A:345:GLN:HB3	1:A:459:MET:HE1	1.71	0.72
1:A:242:LYS:C	1:A:243:ILE:HG13	2.12	0.72
1:A:293:ILE:O	1:A:296:VAL:CG2	2.36	0.72
1:A:428:MET:HA	1:A:432:ASN:HB3	1.70	0.71
1:A:118:VAL:HA	1:A:196:THR:HG22	1.74	0.69
1:A:23:LEU:HD11	1:A:210:ALA:HA	1.74	0.69
1:A:161:GLY:HA2	1:A:393:VAL:HG21	1.75	0.69
1:A:364:TYR:O	1:A:366:GLN:NE2	2.25	0.68
1:A:269:ARG:HH12	1:A:410:ILE:HD11	1.56	0.68
1:A:258:HIS:O	1:A:262:HIS:N	2.28	0.67
1:A:227:LEU:HB3	1:A:232:LYS:HB3	1.77	0.67
1:A:244:MET:HG3	1:A:248:LEU:HD12	1.78	0.66
1:A:102:SER:OG	1:A:203:PHE:HD1	1.66	0.66
1:A:341:ARG:NH1	1:A:397:GLU:OE2	2.29	0.66
1:A:349:ALA:HB2	1:A:387:TRP:HE1	1.60	0.65
1:A:259:SER:OG	1:A:401:ASN:ND2	2.31	0.64
1:A:289:GLN:HE22	1:A:294:ASN:HD21	1.45	0.64
1:A:459:MET:HG3	1:A:463:VAL:HB	1.80	0.63
1:A:253:VAL:HG12	1:A:257:LYS:HE2	1.81	0.62
1:A:56:LEU:O	1:A:60:CYS:N	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:THR:HB	1:A:271:LEU:HD13	1.82	0.62
1:A:296:VAL:HG21	1:A:379:TYR:HE2	1.65	0.61
1:A:271:LEU:O	1:A:271:LEU:HG	1.99	0.61
1:A:10:ILE:HB	1:A:243:ILE:HG21	1.82	0.61
1:A:49:SER:O	1:A:51:SER:N	2.35	0.60
1:A:281:GLY:O	1:A:285:SER:N	2.33	0.60
1:A:84:ARG:HD3	1:A:149:MET:HE2	1.84	0.60
1:A:209:PRO:O	1:A:213:PHE:N	2.33	0.60
1:A:299:TYR:O	1:A:303:VAL:HG22	2.01	0.60
1:A:88:LEU:HD22	1:A:213:PHE:HZ	1.66	0.60
1:A:285:SER:O	1:A:288:GLN:N	2.22	0.59
1:A:228:MET:HE1	1:A:233:GLN:HA	1.84	0.59
1:A:88:LEU:HD22	1:A:213:PHE:CZ	2.38	0.59
1:A:300:ALA:N	1:A:301:PRO:CD	2.65	0.59
1:A:16:VAL:HA	1:A:19:LEU:HD12	1.85	0.58
1:A:275:VAL:O	1:A:275:VAL:HG13	2.01	0.58
1:A:279:VAL:HG12	1:A:283:MET:HG2	1.84	0.58
1:A:160:ARG:NH2	1:A:469:LYS:O	2.36	0.57
1:A:237:GLU:HA	1:A:240:LEU:HD12	1.86	0.57
1:A:288:GLN:HG3	1:A:391:CYS:SG	2.44	0.57
1:A:296:VAL:HG23	1:A:297:LEU:HD12	1.85	0.57
1:A:46:GLN:HE22	1:A:123:ALA:HB1	1.71	0.56
1:A:226:TRP:HD1	1:A:227:LEU:HD23	1.71	0.56
1:A:262:HIS:HA	1:A:265:LYS:HB2	1.88	0.56
1:A:135:ILE:HA	1:A:138:ILE:HD12	1.87	0.56
1:A:255:GLU:HG2	1:A:472:GLU:HG3	1.86	0.56
1:A:225:ARG:NE	1:A:472:GLU:OE2	2.37	0.56
1:A:9:TYR:HD2	1:A:243:ILE:CG1	2.06	0.55
1:A:290:PHE:HD2	1:A:451:MET:HE1	1.71	0.55
1:A:421:PHE:HA	1:A:424:TRP:HB3	1.87	0.55
1:A:56:LEU:HA	1:A:59:PHE:HB3	1.88	0.55
1:A:249:ALA:C	1:A:251:GLN:H	2.14	0.55
1:A:350:LEU:O	1:A:353:ALA:N	2.37	0.54
1:A:399:PHE:HB2	1:A:404:ARG:HD3	1.88	0.54
1:A:14:THR:OG1	1:A:163:LEU:HD11	2.08	0.54
1:A:269:ARG:HA	1:A:269:ARG:NH2	2.21	0.54
1:A:83:GLY:O	1:A:87:SER:N	2.36	0.54
1:A:249:ALA:O	1:A:253:VAL:N	2.34	0.54
1:A:375:SER:O	1:A:379:TYR:N	2.36	0.54
1:A:438:HIS:CD2	1:A:439:PHE:CD1	2.96	0.54
1:A:415:GLN:O	1:A:419:ASN:N	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLY:O	1:A:326:LEU:N	2.39	0.53
1:A:235:GLN:O	1:A:239:ILE:HG13	2.08	0.53
1:A:390:VAL:HA	1:A:393:VAL:HG12	1.91	0.53
1:A:300:ALA:H	1:A:301:PRO:HD2	1.74	0.53
1:A:49:SER:HB3	1:A:52:ALA:HB3	1.92	0.52
1:A:9:TYR:CE2	1:A:243:ILE:CG1	2.92	0.52
1:A:285:SER:O	1:A:287:PHE:N	2.42	0.52
1:A:348:GLY:HA3	1:A:386:SER:HB3	1.92	0.52
1:A:209:PRO:HA	1:A:212:LEU:HB3	1.92	0.52
1:A:238:GLY:O	1:A:242:LYS:HE3	2.09	0.52
1:A:223:SER:O	1:A:226:TRP:HB3	2.10	0.52
1:A:269:ARG:NH1	1:A:410:ILE:CD1	2.70	0.51
1:A:284:LEU:HD11	1:A:394:LEU:HD13	1.93	0.51
1:A:310:SER:O	1:A:313:ILE:HG22	2.11	0.51
1:A:154:LEU:O	1:A:244:MET:HE1	2.10	0.51
1:A:142:LEU:O	1:A:146:LEU:HG	2.11	0.51
1:A:421:PHE:O	1:A:425:THR:N	2.43	0.51
1:A:22:LEU:HA	1:A:170:ALA:O	2.11	0.51
1:A:342:LYS:HB2	1:A:343:PRO:HD3	1.92	0.51
1:A:9:TYR:CE2	1:A:243:ILE:HG12	2.43	0.50
1:A:249:ALA:C	1:A:251:GLN:N	2.69	0.50
1:A:153:GLU:O	1:A:225:ARG:NH1	2.45	0.50
1:A:176:LEU:HD12	1:A:326:LEU:HD22	1.93	0.50
1:A:8:SER:O	1:A:12:SER:OG	2.24	0.50
1:A:294:ASN:HB3	1:A:298:TYR:CD2	2.42	0.49
1:A:248:LEU:HD22	1:A:251:GLN:CD	2.35	0.49
1:A:393:VAL:O	1:A:397:GLU:HG2	2.12	0.49
1:A:403:ILE:O	1:A:405:GLY:N	2.46	0.49
1:A:122:LEU:HA	1:A:125:TYR:CD1	2.48	0.49
1:A:194:LEU:O	1:A:199:TRP:N	2.45	0.49
1:A:95:PHE:O	1:A:99:GLY:N	2.45	0.49
1:A:99:GLY:HA3	1:A:207:CYS:SG	2.53	0.49
1:A:299:TYR:O	1:A:303:VAL:HG13	2.12	0.49
1:A:348:GLY:O	1:A:352:MET:HG3	2.13	0.49
1:A:228:MET:N	1:A:228:MET:SD	2.85	0.49
1:A:295:VAL:HG23	1:A:299:TYR:CD2	2.47	0.49
1:A:403:ILE:HG22	1:A:406:LYS:NZ	2.27	0.49
1:A:202:MET:O	1:A:205:SER:OG	2.27	0.48
1:A:52:ALA:O	1:A:55:SER:OG	2.32	0.48
1:A:347:ILE:HA	1:A:350:LEU:HD12	1.95	0.48
1:A:79:SER:O	1:A:84:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLY:O	1:A:280:ILE:CG1	2.53	0.48
1:A:168:GLN:HG3	1:A:171:ILE:HD12	1.96	0.48
1:A:81:ARG:HG3	1:A:82:PHE:CD1	2.49	0.47
1:A:249:ALA:O	1:A:251:GLN:N	2.47	0.47
1:A:14:THR:O	1:A:18:THR:HG23	2.15	0.47
1:A:238:GLY:O	1:A:241:ARG:N	2.47	0.47
1:A:224:PRO:HA	1:A:227:LEU:HD12	1.97	0.47
1:A:288:GLN:O	1:A:289:GLN:HG2	2.15	0.47
1:A:162:LYS:HB2	1:A:337:ASP:OD2	2.14	0.47
1:A:403:ILE:HD12	1:A:407:ALA:HB2	1.97	0.47
1:A:438:HIS:HD2	1:A:439:PHE:CD1	2.33	0.47
1:A:196:THR:O	1:A:199:TRP:NE1	2.47	0.46
1:A:459:MET:HG3	1:A:463:VAL:CB	2.46	0.46
1:A:295:VAL:O	1:A:295:VAL:HG22	2.14	0.46
1:A:471:LEU:HD12	1:A:471:LEU:H	1.80	0.46
1:A:98:SER:O	1:A:102:SER:HB3	2.15	0.46
1:A:164:VAL:HB	1:A:393:VAL:HG23	1.98	0.46
1:A:16:VAL:O	1:A:19:LEU:HB2	2.16	0.46
1:A:110:THR:OG1	1:A:111:SER:N	2.49	0.46
1:A:348:GLY:HA3	1:A:386:SER:CB	2.46	0.46
1:A:37:SER:O	1:A:41:VAL:N	2.50	0.45
1:A:278:ILE:O	1:A:282:VAL:HG23	2.17	0.45
1:A:67:GLY:O	1:A:71:GLY:N	2.36	0.45
1:A:145:MET:HE3	1:A:408:LEU:HD23	1.99	0.45
1:A:447:ILE:O	1:A:451:MET:HG3	2.16	0.45
1:A:167:ASN:O	1:A:170:ALA:N	2.42	0.45
1:A:84:ARG:NE	1:A:153:GLU:OE1	2.50	0.44
1:A:316:LEU:O	1:A:320:ILE:HG12	2.18	0.44
1:A:397:GLU:C	1:A:399:PHE:H	2.26	0.44
1:A:126:VAL:HB	1:A:127:PRO:HD3	1.99	0.44
1:A:314:ALA:O	1:A:317:GLN:HB3	2.17	0.44
1:A:341:ARG:HD2	1:A:390:VAL:HG13	1.99	0.44
1:A:289:GLN:O	1:A:292:GLY:N	2.43	0.44
1:A:356:MET:HB3	1:A:445:TYR:O	2.18	0.44
1:A:9:TYR:HE2	1:A:243:ILE:HD11	1.83	0.44
1:A:70:ILE:O	1:A:74:LEU:HD13	2.17	0.44
1:A:434:TRP:O	1:A:438:HIS:N	2.35	0.44
1:A:341:ARG:CG	1:A:341:ARG:HH11	2.31	0.43
1:A:364:TYR:CD1	1:A:440:HIS:HA	2.53	0.43
1:A:213:PHE:O	1:A:217:LEU:HG	2.19	0.43
1:A:233:GLN:O	1:A:237:GLU:N	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TYR:OH	1:A:423:SER:O	2.37	0.43
1:A:325:ASN:O	1:A:329:THR:OG1	2.21	0.43
1:A:26:TYR:CZ	1:A:178:VAL:HB	2.54	0.43
1:A:401:ASN:OD1	1:A:404:ARG:NH2	2.52	0.43
1:A:269:ARG:HH11	1:A:410:ILE:HD11	1.80	0.43
1:A:275:VAL:HG22	1:A:278:ILE:HD12	2.01	0.43
1:A:285:SER:O	1:A:286:ILE:C	2.62	0.43
1:A:176:LEU:CD1	1:A:326:LEU:HD22	2.49	0.43
1:A:269:ARG:C	1:A:269:ARG:HD3	2.44	0.43
1:A:275:VAL:CG2	1:A:278:ILE:HD12	2.49	0.42
1:A:341:ARG:HD3	1:A:341:ARG:HA	1.56	0.42
1:A:192:SER:O	1:A:196:THR:N	2.49	0.42
1:A:342:LYS:NZ	1:A:463:VAL:O	2.40	0.42
1:A:25:GLY:HA3	1:A:171:ILE:O	2.20	0.42
1:A:27:ASP:O	1:A:133:ARG:NH1	2.48	0.42
1:A:374:LEU:O	1:A:378:PHE:N	2.44	0.42
1:A:43:VAL:HG12	1:A:56:LEU:HD11	2.01	0.42
1:A:101:GLY:HA3	1:A:132:TYR:HB3	2.01	0.42
1:A:277:VAL:CG1	1:A:478:TRP:CZ2	3.03	0.42
1:A:469:LYS:HB3	1:A:473:GLU:HB2	2.00	0.42
1:A:134:ILE:O	1:A:138:ILE:HG13	2.19	0.42
1:A:288:GLN:CG	1:A:391:CYS:SG	3.07	0.42
1:A:129:PHE:O	1:A:133:ARG:N	2.52	0.42
1:A:292:GLY:O	1:A:379:TYR:OH	2.34	0.42
1:A:22:LEU:HB2	1:A:170:ALA:HB1	2.02	0.42
1:A:288:GLN:C	1:A:289:GLN:HG2	2.44	0.42
1:A:8:SER:HA	1:A:11:PHE:HB2	2.01	0.42
1:A:27:ASP:OD1	1:A:133:ARG:NH1	2.53	0.41
1:A:155:ALA:HB2	1:A:163:LEU:HD23	2.02	0.41
1:A:345:GLN:HB3	1:A:459:MET:CE	2.45	0.41
1:A:272:MET:HE3	1:A:277:VAL:HG23	2.03	0.41
1:A:353:ALA:HA	1:A:449:GLY:HA2	2.02	0.41
1:A:151:ILE:O	1:A:155:ALA:N	2.47	0.41
1:A:248:LEU:O	1:A:252:ALA:N	2.53	0.41
1:A:21:GLY:HA3	1:A:167:ASN:OD1	2.20	0.41
1:A:247:THR:C	1:A:249:ALA:N	2.78	0.41
1:A:300:ALA:O	1:A:304:PHE:CD1	2.74	0.41
1:A:10:ILE:O	1:A:14:THR:OG1	2.28	0.41
1:A:147:SER:HB2	1:A:148:PRO:HD3	2.02	0.41
1:A:272:MET:H	1:A:272:MET:HG2	1.78	0.40
1:A:315:TRP:O	1:A:319:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:MET:O	1:A:379:TYR:HB3	2.21	0.40
1:A:284:LEU:O	1:A:387:TRP:HZ3	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	473/518 (91%)	379 (80%)	74 (16%)	20 (4%)	2	20

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	285	SER
1	A	286	ILE
1	A	309	ALA
1	A	404	ARG
1	A	48	LEU
1	A	250	THR
1	A	351	GLY
1	A	113	ASN
1	A	49	SER
1	A	115	ASP
1	A	222	GLU
1	A	269	ARG
1	A	338	LYS
1	A	275	VAL
1	A	388	GLY
1	A	280	ILE
1	A	253	VAL
1	A	243	ILE

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Mol	Chain	Res	Type
1	A	398	ILE

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	376/420 (90%)	348 (93%)	28 (7%)	13	39

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	37	SER
1	A	39	ASN
1	A	50	GLU
1	A	54	ASN
1	A	107	LEU
1	A	118	VAL
1	A	194	LEU
1	A	243	ILE
1	A	248	LEU
1	A	266	THR
1	A	269	ARG
1	A	270	LEU
1	A	272	MET
1	A	273	PHE
1	A	275	VAL
1	A	277	VAL
1	A	279	VAL
1	A	288	GLN
1	A	296	VAL
1	A	312	ASP
1	A	315	TRP
1	A	336	VAL
1	A	341	ARG
1	A	406	LYS

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Mol	Chain	Res	Type
1	A	438	HIS
1	A	444	SER
1	A	467	LYS

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	ASN
1	A	46	GLN
1	A	258	HIS
1	A	288	GLN
1	A	289	GLN
1	A	294	ASN
1	A	366	GLN
1	A	415	GLN
1	A	438	HIS

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 [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 ⓘ

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	475/518 (91%)	1.00	79 (16%) 4 6	79, 117, 169, 191	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	GLY	7.0
1	A	276	GLY	7.0
1	A	294	ASN	6.9
1	A	201	TYR	5.5
1	A	298	TYR	5.4
1	A	297	LEU	5.4
1	A	200	ARG	5.1
1	A	293	ILE	4.9
1	A	330	VAL	4.4
1	A	468	GLY	4.4
1	A	269	ARG	4.4
1	A	204	ALA	4.3
1	A	40	THR	4.2
1	A	117	THR	4.1
1	A	288	GLN	4.1
1	A	339	PHE	3.9
1	A	258	HIS	3.8
1	A	9	TYR	3.8
1	A	169	PHE	3.6
1	A	107	LEU	3.5
1	A	42	PHE	3.5
1	A	289	GLN	3.5
1	A	270	LEU	3.4
1	A	197	ASP	3.3
1	A	199	TRP	3.2
1	A	158	HIS	3.2
1	A	292	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	304	PHE	3.2
1	A	275	VAL	3.1
1	A	24	PHE	3.0
1	A	467	LYS	3.0
1	A	221	PRO	3.0
1	A	124	GLY	3.0
1	A	305	LYS	3.0
1	A	296	VAL	3.0
1	A	266	THR	2.9
1	A	307	LEU	2.9
1	A	206	GLU	2.9
1	A	370	ILE	2.8
1	A	25	GLY	2.8
1	A	168	GLN	2.8
1	A	261	ASP	2.8
1	A	104	TRP	2.8
1	A	279	VAL	2.8
1	A	65	LEU	2.8
1	A	231	GLY	2.8
1	A	15	LEU	2.7
1	A	56	LEU	2.7
1	A	26	TYR	2.6
1	A	130	VAL	2.6
1	A	410	ILE	2.6
1	A	420	TYR	2.6
1	A	366	GLN	2.6
1	A	331	LEU	2.5
1	A	280	ILE	2.5
1	A	469	LYS	2.5
1	A	125	TYR	2.5
1	A	254	GLN	2.5
1	A	191	ALA	2.4
1	A	164	VAL	2.4
1	A	393	VAL	2.4
1	A	479	GLU	2.4
1	A	315	TRP	2.3
1	A	267	GLY	2.3
1	A	265	LYS	2.3
1	A	272	MET	2.2
1	A	277	VAL	2.2
1	A	215	MET	2.2
1	A	459	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	462	PHE	2.2
1	A	274	GLY	2.1
1	A	396	SER	2.1
1	A	28	THR	2.1
1	A	242	LYS	2.1
1	A	385	MET	2.1
1	A	302	GLU	2.1
1	A	365	THR	2.1
1	A	34	THR	2.0
1	A	82	PHE	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.