



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:41 PM UTC

PDB ID : 2WCS / pdb_00002wcs
Title : Crystal Structure of Debranching enzyme from Nostoc punctiforme (NPDE)
Authors : Dumbrepatil, A.B.; Choi, J.H.; Nam, S.H.; Park, K.H.; Woo, E.J.
Deposited on : 2009-03-16
Resolution : 2.80 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

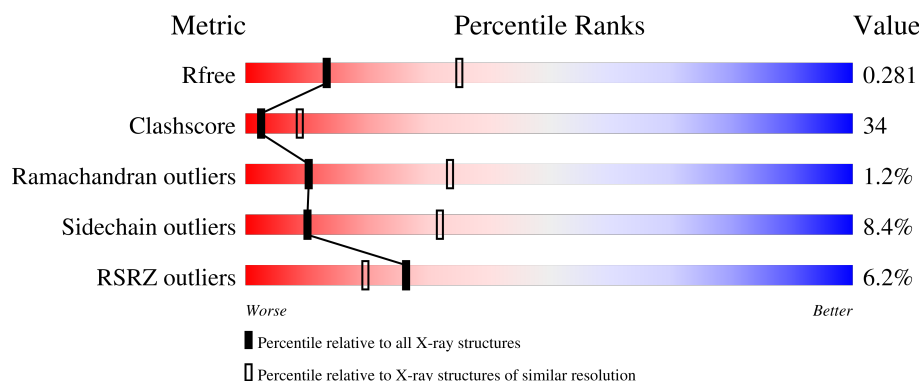
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	488	6% 50% 42% 6% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3968 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 ALPHA AMYLASE, CATALYTIC REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	2
			3922	2526	662	727	7			

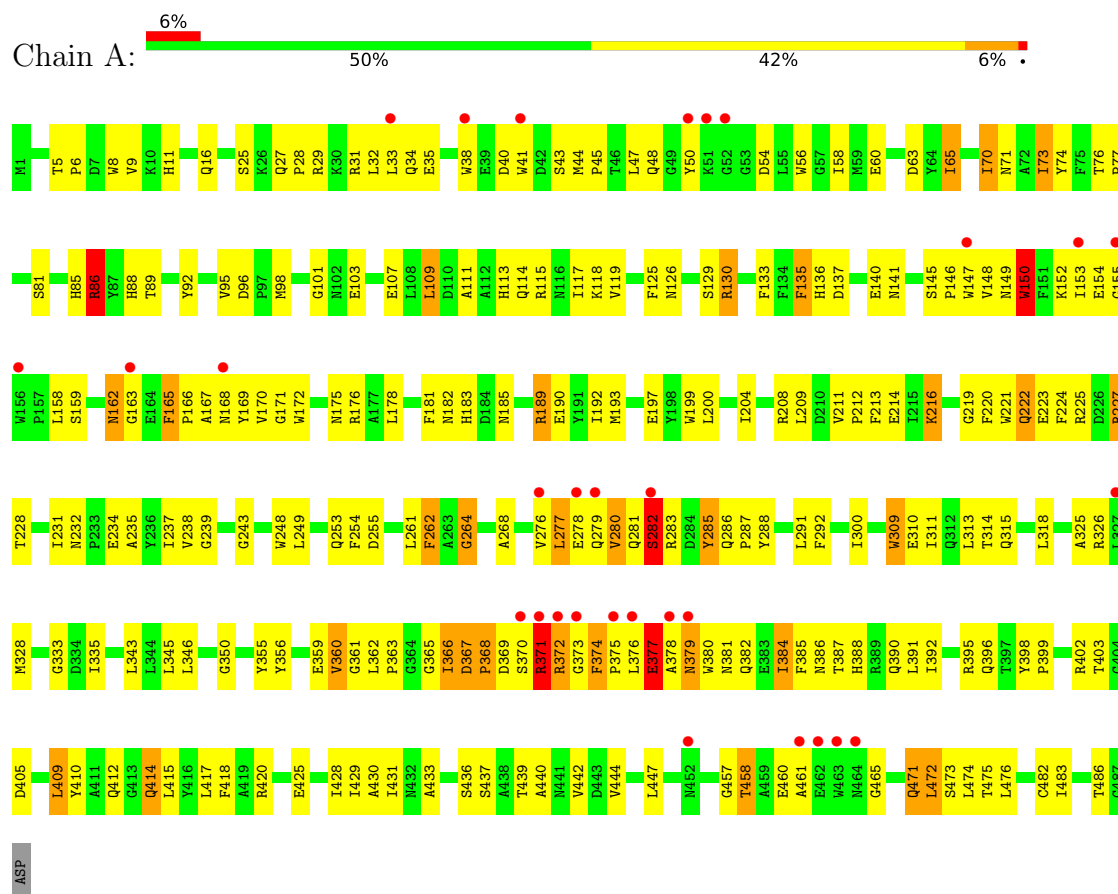
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	46	Total	O	0	0
			46	46		

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: ALPHA AMYLASE, CATALYTIC REGION



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.73Å 93.73Å 257.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.88 – 2.80 29.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.88-2.80) 94.1 (29.88-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.44 (at 2.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.224 , 0.284 0.221 , 0.281	Depositor DCC
R_{free} test set	785 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3968	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	1/4042 (0.0%)	0.84	9/5515 (0.2%)

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
1	A	2	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	THR	C-N	-5.76	1.25	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	PHE	N-CA-C	-6.56	104.05	111.14
1	A	150	TRP	N-CA-C	-6.18	105.53	114.12
1	A	398	TYR	CA-C-N	5.94	125.81	119.28
1	A	398	TYR	C-N-CA	5.94	125.81	119.28
1	A	387	THR	N-CA-C	-5.73	104.94	111.07
1	A	255	ASP	N-CA-C	-5.17	106.97	113.28
1	A	264	GLY	CA-C-N	5.14	124.32	118.97
1	A	264	GLY	C-N-CA	5.14	124.32	118.97
1	A	262	PHE	N-CA-C	-5.02	107.28	113.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	281	GLN	CA

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Mol	Chain	Res	Type	Atom
1	A	379	ASN	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	PRO	Peptide
1	A	280	VAL	Peptide
1	A	282	SER	Peptide
1	A	366	ILE	Peptide
1	A	367	ASP	Peptide
1	A	369	ASP	Peptide
1	A	371	ARG	Peptide
1	A	374	PHE	Peptide
1	A	377	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3922	0	3726	262	0
2	A	46	0	0	1	0
All	All	3968	0	3726	262	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 34.

All (262) 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:377:GLU:O	1:A:379:ASN:HA	1.45	1.17
1:A:155:GLY:H	1:A:168:ASN:HB3	1.06	1.11
1:A:367:ASP:HB3	1:A:368:PRO:HD3	1.31	1.09
1:A:193:MET:HE1	1:A:224:PHE:HA	1.30	1.09
1:A:367:ASP:CG	1:A:368:PRO:HB3	1.82	1.04
1:A:362:LEU:HD11	1:A:373:GLY:HA3	1.46	0.96
1:A:367:ASP:OD2	1:A:368:PRO:HB3	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LEU:HD11	1:A:483:ILE:HD11	1.48	0.94
1:A:360:VAL:HG13	1:A:380:TRP:HA	1.47	0.94
1:A:228:THR:HG21	1:A:237:ILE:HD11	1.48	0.93
1:A:31:ARG:NH2	1:A:31:ARG:HB2	1.83	0.93
1:A:155:GLY:N	1:A:168:ASN:HB3	1.84	0.92
1:A:379:ASN:O	1:A:380:TRP:HD1	1.55	0.88
1:A:361:GLY:N	1:A:384:ILE:HD11	1.91	0.85
1:A:73:ILE:HD11	1:A:119:VAL:HG22	1.60	0.84
1:A:31:ARG:HB2	1:A:31:ARG:HH21	1.41	0.83
1:A:367:ASP:HB3	1:A:368:PRO:CD	2.08	0.83
1:A:76:THR:HB	1:A:77:PRO:HD2	1.59	0.83
1:A:189:ARG:O	1:A:193:MET:HG2	1.79	0.82
1:A:54:ASP:OD1	1:A:56:TRP:HB2	1.79	0.81
1:A:11:HIS:HD2	1:A:402:ARG:HE	1.28	0.81
1:A:461:ALA:HB3	1:A:475:THR:N	1.95	0.80
1:A:65:ILE:HG22	1:A:70:ILE:CG1	2.12	0.80
1:A:366:ILE:CG2	1:A:367:ASP:H	1.95	0.79
1:A:280:VAL:HG12	1:A:282:SER:N	1.99	0.78
1:A:377:GLU:C	1:A:379:ASN:HA	2.08	0.78
1:A:360:VAL:HG13	1:A:380:TRP:CA	2.15	0.77
1:A:154:GLU:N	1:A:168:ASN:O	2.18	0.76
1:A:366:ILE:HG23	1:A:367:ASP:H	1.50	0.76
1:A:366:ILE:HG23	1:A:367:ASP:N	2.01	0.75
1:A:76:THR:HB	1:A:77:PRO:CD	2.17	0.74
1:A:367:ASP:OD2	1:A:368:PRO:CB	2.36	0.74
1:A:193:MET:HE2	1:A:227:ARG:HD3	1.69	0.73
1:A:279:GLN:HB3	1:A:325:ALA:CB	2.19	0.73
1:A:171:GLY:HA3	1:A:175:ASN:O	1.89	0.73
1:A:360:VAL:CG1	1:A:380:TRP:HA	2.17	0.73
1:A:27:GLN:HB2	1:A:28:PRO:HD2	1.70	0.72
1:A:32:LEU:HB3	1:A:47:LEU:HD21	1.71	0.72
1:A:159:SER:OG	1:A:162:ASN:HB3	1.90	0.71
1:A:193:MET:HE1	1:A:224:PHE:CA	2.16	0.70
1:A:153:ILE:HD11	1:A:158:LEU:HD21	1.73	0.70
1:A:472:LEU:HD23	1:A:473:SER:N	2.06	0.70
1:A:377:GLU:O	1:A:379:ASN:CA	2.32	0.70
1:A:376:LEU:O	1:A:377:GLU:N	2.25	0.69
1:A:163:GLY:HA2	1:A:176:ARG:NH1	2.07	0.69
1:A:5:THR:HB	1:A:314:THR:HG21	1.74	0.69
1:A:461:ALA:O	1:A:474:LEU:HA	1.93	0.69
1:A:276:VAL:HG12	1:A:278:GLU:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:SER:O	1:A:45:PRO:HD3	1.94	0.67
1:A:281:GLN:H	1:A:366:ILE:HD11	1.58	0.67
1:A:366:ILE:CG2	1:A:367:ASP:N	2.55	0.67
1:A:172:TRP:HZ3	1:A:214:GLU:HG3	1.60	0.66
1:A:277:LEU:O	1:A:277:LEU:HD12	1.95	0.66
1:A:414:GLN:HG3	1:A:433:ALA:HB3	1.77	0.66
1:A:367:ASP:CG	1:A:368:PRO:CB	2.66	0.66
1:A:219:GLY:O	1:A:222:GLN:HG2	1.95	0.66
1:A:279:GLN:HB3	1:A:325:ALA:HB2	1.77	0.66
1:A:197:GLU:HG2	1:A:231:ILE:HD11	1.78	0.65
1:A:362:LEU:HD23	1:A:363:PRO:O	1.97	0.65
1:A:379:ASN:N	1:A:379:ASN:OD1	2.30	0.65
1:A:360:VAL:CG1	1:A:360:VAL:O	2.46	0.63
1:A:460:GLU:CD	1:A:461:ALA:H	2.06	0.63
1:A:292:PHE:HA	1:A:414:GLN:HE22	1.62	0.62
1:A:429:ILE:HD12	1:A:483:ILE:HG13	1.82	0.62
1:A:310:GLU:HG2	2:A:2034:HOH:O	1.99	0.62
1:A:461:ALA:HB3	1:A:475:THR:H	1.65	0.61
1:A:16:GLN:HB2	1:A:74:TYR:CZ	2.36	0.61
1:A:193:MET:CE	1:A:227:ARG:HD3	2.29	0.61
1:A:167:ALA:HB1	1:A:169:TYR:CE2	2.35	0.61
1:A:70:ILE:HD12	1:A:70:ILE:C	2.25	0.61
1:A:71:ASN:C	1:A:117:ILE:HG23	2.26	0.61
1:A:379:ASN:O	1:A:380:TRP:CD1	2.46	0.61
1:A:41:TRP:HA	1:A:44:MET:HE3	1.82	0.60
1:A:147:TRP:O	1:A:150:TRP:HB2	2.01	0.60
1:A:379:ASN:C	1:A:380:TRP:CD1	2.79	0.60
1:A:65:ILE:HG22	1:A:70:ILE:HG13	1.84	0.60
1:A:133:PHE:O	1:A:136:HIS:HB3	2.01	0.60
1:A:54:ASP:O	1:A:58:ILE:HD13	2.01	0.60
1:A:379:ASN:C	1:A:380:TRP:HD1	2.09	0.59
1:A:211:VAL:HG12	1:A:211:VAL:O	2.02	0.59
1:A:182:ASN:ND2	1:A:185:ASN:HB2	2.16	0.59
1:A:73:ILE:CD1	1:A:119:VAL:HG22	2.30	0.59
1:A:418:PHE:CE1	1:A:429:ILE:HB	2.36	0.59
1:A:41:TRP:NE1	1:A:48:GLN:HA	2.18	0.58
1:A:155:GLY:H	1:A:168:ASN:CB	1.99	0.58
1:A:165:PHE:CD1	1:A:165:PHE:N	2.69	0.58
1:A:71:ASN:O	1:A:117:ILE:HA	2.03	0.58
1:A:249:LEU:HD13	1:A:311:ILE:HG21	1.86	0.58
1:A:377:GLU:N	1:A:377:GLU:CD	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:TRP:CZ3	1:A:313:LEU:HD11	2.39	0.58
1:A:417:LEU:HG	1:A:430:ALA:HB2	1.87	0.57
1:A:152:LYS:HE3	1:A:181:PHE:O	2.03	0.57
1:A:211:VAL:HG13	1:A:213:PHE:CZ	2.40	0.57
1:A:285:TYR:N	1:A:285:TYR:CD2	2.71	0.57
1:A:167:ALA:N	1:A:176:ARG:NH2	2.53	0.57
1:A:367:ASP:OD2	1:A:368:PRO:CA	2.53	0.57
1:A:277:LEU:O	1:A:277:LEU:CD1	2.53	0.57
1:A:109:LEU:HD22	1:A:113:HIS:CE1	2.40	0.56
1:A:384:ILE:HG13	1:A:385:PHE:N	2.20	0.56
1:A:32:LEU:H	1:A:47:LEU:HD23	1.70	0.56
1:A:382:GLN:O	1:A:386:ASN:ND2	2.39	0.56
1:A:280:VAL:HG12	1:A:282:SER:HB3	1.88	0.56
1:A:153:ILE:HG23	1:A:153:ILE:O	2.06	0.56
1:A:211:VAL:HG13	1:A:213:PHE:CE1	2.42	0.55
1:A:211:VAL:CG1	1:A:214:GLU:HG2	2.37	0.55
1:A:165:PHE:N	1:A:165:PHE:HD1	2.05	0.55
1:A:172:TRP:CZ3	1:A:214:GLU:HG3	2.40	0.55
1:A:162:ASN:C	1:A:162:ASN:HD22	2.14	0.55
1:A:149:ASN:O	1:A:185:ASN:ND2	2.40	0.55
1:A:367:ASP:CB	1:A:368:PRO:CD	2.82	0.54
1:A:461:ALA:O	1:A:474:LEU:HD23	2.07	0.54
1:A:248:TRP:HA	1:A:253:GLN:NE2	2.23	0.54
1:A:356:TYR:CD1	1:A:375:PRO:HG3	2.42	0.54
1:A:439:THR:HA	1:A:474:LEU:O	2.07	0.54
1:A:98:MET:HE2	1:A:98:MET:HA	1.89	0.54
1:A:283:ARG:HD2	1:A:283:ARG:O	2.07	0.54
1:A:211:VAL:HG12	1:A:214:GLU:HG2	1.89	0.54
1:A:367:ASP:OD2	1:A:368:PRO:HA	2.08	0.54
1:A:360:VAL:HG13	1:A:380:TRP:CB	2.37	0.53
1:A:280:VAL:HG12	1:A:282:SER:CB	2.39	0.53
1:A:345:LEU:HD13	1:A:346:LEU:HD23	1.91	0.53
1:A:25:SER:HB2	1:A:60:GLU:OE2	2.09	0.53
1:A:73:ILE:HD13	1:A:73:ILE:H	1.74	0.53
1:A:209:LEU:O	1:A:212:PRO:HD3	2.09	0.52
1:A:417:LEU:HD21	1:A:474:LEU:HD12	1.91	0.52
1:A:65:ILE:CG2	1:A:70:ILE:HD11	2.39	0.52
1:A:461:ALA:CB	1:A:475:THR:HB	2.39	0.52
1:A:405:ASP:O	1:A:420:ARG:HA	2.09	0.52
1:A:56:TRP:HZ3	1:A:107:GLU:OE2	1.92	0.52
1:A:309:TRP:CE3	1:A:313:LEU:HD11	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD12	1:A:391:LEU:CB	2.38	0.52
1:A:280:VAL:HG12	1:A:282:SER:CA	2.39	0.52
1:A:58:ILE:H	1:A:58:ILE:CD1	2.22	0.52
1:A:457:GLY:HA3	1:A:482:CYS:HA	1.90	0.52
1:A:6:PRO:HB2	1:A:9:VAL:HG23	1.92	0.51
1:A:472:LEU:HD23	1:A:473:SER:H	1.71	0.51
1:A:234:GLU:OE1	1:A:234:GLU:HA	2.10	0.51
1:A:335:ILE:N	1:A:335:ILE:HD12	2.26	0.51
1:A:285:TYR:N	1:A:285:TYR:HD2	2.08	0.51
1:A:356:TYR:HD1	1:A:375:PRO:HG3	1.74	0.51
1:A:197:GLU:HG2	1:A:231:ILE:CD1	2.41	0.51
1:A:343:LEU:HD11	1:A:483:ILE:CD1	2.32	0.51
1:A:58:ILE:H	1:A:58:ILE:HD12	1.77	0.50
1:A:197:GLU:HA	1:A:231:ILE:HD12	1.94	0.50
1:A:223:GLU:HG2	1:A:227:ARG:HD2	1.94	0.50
1:A:65:ILE:HG22	1:A:70:ILE:CD1	2.41	0.50
1:A:65:ILE:HG22	1:A:70:ILE:HD11	1.93	0.50
1:A:372:ARG:HG2	1:A:373:GLY:N	2.24	0.49
1:A:193:MET:HE2	1:A:223:GLU:HG2	1.94	0.49
1:A:292:PHE:HA	1:A:414:GLN:NE2	2.27	0.49
1:A:285:TYR:HD2	1:A:285:TYR:H	1.60	0.49
1:A:58:ILE:HD12	1:A:58:ILE:N	2.27	0.48
1:A:346:LEU:HD12	1:A:391:LEU:HB2	1.94	0.48
1:A:95:VAL:HB	1:A:101:GLY:C	2.38	0.48
1:A:178:LEU:N	1:A:178:LEU:HD22	2.28	0.48
1:A:199:TRP:O	1:A:204:ILE:HG12	2.12	0.48
1:A:410:TYR:CZ	1:A:412:GLN:HB2	2.48	0.48
1:A:309:TRP:HH2	1:A:403:THR:O	1.97	0.48
1:A:181:PHE:HB2	1:A:183:HIS:CE1	2.49	0.48
1:A:200:LEU:HD11	1:A:228:THR:HG23	1.96	0.47
1:A:31:ARG:HB2	1:A:31:ARG:CZ	2.44	0.47
1:A:193:MET:HE2	1:A:227:ARG:CD	2.41	0.47
1:A:81:SER:OG	1:A:86:ARG:HA	2.14	0.47
1:A:209:LEU:HD12	1:A:254:PHE:CE1	2.50	0.47
1:A:264:GLY:O	1:A:287:PRO:HA	2.14	0.47
1:A:279:GLN:NE2	1:A:365:GLY:HA2	2.29	0.47
1:A:197:GLU:CG	1:A:231:ILE:HD11	2.44	0.47
1:A:378:ALA:HA	1:A:380:TRP:CD1	2.50	0.47
1:A:381:ASN:HB3	1:A:384:ILE:HG12	1.97	0.47
1:A:444:VAL:HG23	1:A:444:VAL:O	2.15	0.47
1:A:415:LEU:HD23	1:A:440:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:PRO:HD2	1:A:425:GLU:OE1	2.15	0.47
1:A:76:THR:CB	1:A:77:PRO:CD	2.83	0.46
1:A:130:ARG:HA	1:A:135:PHE:CD2	2.51	0.46
1:A:360:VAL:O	1:A:360:VAL:HG12	2.14	0.46
1:A:126:ASN:HA	1:A:183:HIS:CE1	2.51	0.46
1:A:268:ALA:HB3	1:A:291:LEU:HD12	1.96	0.46
1:A:85:HIS:HB3	1:A:88:HIS:CD2	2.50	0.46
1:A:318:LEU:N	1:A:318:LEU:HD23	2.31	0.46
1:A:34:GLN:HG3	1:A:35:GLU:HG2	1.98	0.45
1:A:111:ALA:O	1:A:114:GLN:HG2	2.16	0.45
1:A:141:ASN:HB2	1:A:145:SER:HB2	1.97	0.45
1:A:367:ASP:O	1:A:370:SER:OG	2.30	0.45
1:A:362:LEU:HD13	1:A:375:PRO:HB3	1.98	0.45
1:A:371:ARG:H	1:A:371:ARG:HG2	1.38	0.45
1:A:11:HIS:CD2	1:A:402:ARG:HE	2.19	0.45
1:A:86:ARG:NH2	1:A:96:ASP:OD2	2.50	0.45
1:A:190:GLU:OE2	1:A:227:ARG:NH2	2.49	0.45
1:A:5:THR:HG21	1:A:311:ILE:HD13	1.98	0.45
1:A:154:GLU:HB2	1:A:168:ASN:HB3	1.97	0.45
1:A:350:GLY:O	1:A:395:ARG:NH2	2.49	0.45
1:A:167:ALA:H	1:A:176:ARG:NH2	2.15	0.45
1:A:216:LYS:HE2	1:A:216:LYS:HB3	1.86	0.45
1:A:359:GLU:O	1:A:385:PHE:HA	2.16	0.45
1:A:16:GLN:NE2	1:A:74:TYR:OH	2.49	0.44
1:A:209:LEU:HB2	1:A:239:GLY:HA2	1.99	0.44
1:A:328:MET:HG2	1:A:361:GLY:O	2.16	0.44
1:A:475:THR:C	1:A:476:LEU:HD12	2.41	0.44
1:A:130:ARG:HA	1:A:135:PHE:HD2	1.83	0.44
1:A:209:LEU:HD13	1:A:221:TRP:CZ3	2.53	0.44
1:A:243:GLY:HA2	1:A:261:LEU:HD21	1.97	0.44
1:A:415:LEU:HD12	1:A:431:ILE:O	2.17	0.44
1:A:154:GLU:HB2	1:A:168:ASN:C	2.43	0.44
1:A:286:GLN:C	1:A:288:TYR:H	2.25	0.44
1:A:225:ARG:HD2	1:A:253:GLN:O	2.18	0.44
1:A:88:HIS:C	1:A:129:SER:HB3	2.42	0.44
1:A:386:ASN:O	1:A:390:GLN:HB2	2.18	0.44
1:A:65:ILE:HG22	1:A:70:ILE:HG12	1.96	0.44
1:A:172:TRP:CZ3	1:A:211:VAL:HG11	2.53	0.43
1:A:376:LEU:O	1:A:380:TRP:NE1	2.51	0.43
1:A:125:PHE:HB3	1:A:192:ILE:HD13	2.00	0.43
1:A:211:VAL:HG12	1:A:214:GLU:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD12	1:A:391:LEU:HB3	2.00	0.43
1:A:482:CYS:C	1:A:483:ILE:HD12	2.43	0.43
1:A:282:SER:O	1:A:282:SER:OG	2.30	0.43
1:A:360:VAL:HG13	1:A:360:VAL:O	2.19	0.43
1:A:63:ASP:OD2	1:A:115:ARG:NH2	2.48	0.43
1:A:197:GLU:HA	1:A:231:ILE:CD1	2.48	0.43
1:A:436:SER:O	1:A:437:SER:C	2.61	0.43
1:A:461:ALA:O	1:A:473:SER:O	2.37	0.43
1:A:73:ILE:HD13	1:A:118:LYS:O	2.18	0.43
1:A:311:ILE:O	1:A:315:GLN:HG2	2.19	0.43
1:A:154:GLU:HB2	1:A:168:ASN:CA	2.49	0.43
1:A:361:GLY:H	1:A:384:ILE:HD11	1.78	0.43
1:A:465:GLY:HA3	1:A:471:GLN:OE1	2.19	0.43
1:A:472:LEU:CD2	1:A:473:SER:N	2.78	0.42
1:A:33:LEU:HD22	1:A:33:LEU:H	1.84	0.42
1:A:458:THR:HG23	1:A:458:THR:O	2.18	0.42
1:A:461:ALA:HB2	1:A:475:THR:HB	2.01	0.42
1:A:98:MET:HE2	1:A:98:MET:CA	2.48	0.42
1:A:409:LEU:HB3	1:A:442:VAL:HG11	2.02	0.42
1:A:65:ILE:CG2	1:A:70:ILE:CG1	2.93	0.42
1:A:71:ASN:O	1:A:117:ILE:HG23	2.20	0.42
1:A:333:GLY:O	1:A:335:ILE:HD12	2.20	0.42
1:A:355:TYR:O	1:A:356:TYR:C	2.63	0.42
1:A:326:ARG:CZ	1:A:362:LEU:HD22	2.50	0.42
1:A:428:ILE:C	1:A:429:ILE:HD13	2.45	0.42
1:A:89:THR:HG21	1:A:92:TYR:CE2	2.55	0.41
1:A:152:LYS:HB2	1:A:170:VAL:HB	2.02	0.41
1:A:356:TYR:O	1:A:356:TYR:CG	2.73	0.41
1:A:211:VAL:CG1	1:A:214:GLU:CG	2.98	0.41
1:A:232:ASN:HB3	1:A:235:ALA:HB2	2.01	0.41
1:A:162:ASN:C	1:A:162:ASN:ND2	2.78	0.41
1:A:417:LEU:HG	1:A:430:ALA:CB	2.50	0.41
1:A:420:ARG:HH11	1:A:420:ARG:HG3	1.85	0.41
1:A:137:ASP:OD2	1:A:147:TRP:HZ3	2.03	0.41
1:A:171:GLY:O	1:A:172:TRP:C	2.64	0.41
1:A:392:ILE:O	1:A:396:GLN:HG2	2.21	0.41
1:A:359:GLU:HA	1:A:388:HIS:CD2	2.55	0.41
1:A:262:PHE:CD1	1:A:262:PHE:C	2.98	0.41
1:A:361:GLY:O	1:A:362:LEU:C	2.62	0.41
1:A:8:TRP:CZ3	1:A:118:LYS:HG3	2.56	0.41
1:A:193:MET:HB3	1:A:227:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ALA:HB3	1:A:475:THR:HB	2.03	0.41
1:A:5:THR:CB	1:A:314:THR:HG21	2.46	0.40
1:A:31:ARG:NE	1:A:50:TYR:CD2	2.89	0.40
1:A:48:GLN:NE2	1:A:48:GLN:C	2.79	0.40
1:A:65:ILE:H	1:A:65:ILE:HG12	1.55	0.40
1:A:145:SER:HA	1:A:146:PRO:HD3	1.82	0.40
1:A:148:VAL:HG12	1:A:153:ILE:HG21	2.03	0.40
1:A:40:ASP:O	1:A:43:SER:HB2	2.22	0.40
1:A:366:ILE:HG22	1:A:367:ASP:H	1.79	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	482/488 (99%)	415 (86%)	61 (13%)	6 (1%)	10	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	374	PHE
1	A	368	PRO
1	A	86	ARG
1	A	220	PHE
1	A	458	THR

5.3.2 Protein sidechains [i](#)

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	406/409 (99%)	372 (92%)	34 (8%)	10	32

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	38	TRP
1	A	65	ILE
1	A	70	ILE
1	A	73	ILE
1	A	86	ARG
1	A	103	GLU
1	A	109	LEU
1	A	130	ARG
1	A	140	GLU
1	A	150	TRP
1	A	165	PHE
1	A	189	ARG
1	A	208	ARG
1	A	216	LYS
1	A	222	GLN
1	A	227	ARG
1	A	238	VAL
1	A	277	LEU
1	A	282	SER
1	A	285	TYR
1	A	300	ILE
1	A	309	TRP
1	A	360	VAL
1	A	371	ARG
1	A	372	ARG
1	A	377	GLU
1	A	379	ASN
1	A	384	ILE
1	A	409	LEU
1	A	414	GLN
1	A	447	LEU
1	A	471	GLN
1	A	472	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	11	HIS
1	A	16	GLN
1	A	34	GLN
1	A	48	GLN
1	A	67	ASN
1	A	114	GLN
1	A	127	HIS
1	A	141	ASN
1	A	162	ASN
1	A	168	ASN
1	A	247	GLN
1	A	253	GLN
1	A	301	GLN
1	A	386	ASN
1	A	388	HIS
1	A	412	GLN
1	A	414	GLN
1	A	432	ASN
1	A	470	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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	A	487/488 (99%)	0.21	30 (6%) 26 20	24, 49, 105, 133	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	LEU	5.2
1	A	461	ALA	4.3
1	A	375	PRO	4.1
1	A	373	GLY	4.0
1	A	50	TYR	3.4
1	A	371	ARG	3.2
1	A	463	TRP	3.0
1	A	155	GLY	2.9
1	A	51	LYS	2.8
1	A	278	GLU	2.8
1	A	41	TRP	2.8
1	A	147	TRP	2.8
1	A	38	TRP	2.8
1	A	462	GLU	2.7
1	A	52	GLY	2.7
1	A	464	ASN	2.7
1	A	378	ALA	2.6
1	A	163	GLY	2.5
1	A	370	SER	2.4
1	A	279	GLN	2.4
1	A	282	SER	2.4
1	A	379	ASN	2.3
1	A	327	LEU	2.2
1	A	276	VAL	2.1
1	A	33	LEU	2.1
1	A	372	ARG	2.1
1	A	168	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	452	ASN	2.1
1	A	153	ILE	2.1
1	A	156	TRP	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.