



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:13 AM GMT

PDB ID : 2WC7
Title : CRYSTAL STRUCTURE OF NOSTOC PUNCTIFORME DEBRANCHING
ENZYME(NPDE)(ACARBOSE SOAKED)
Authors : Dumbrepatil, A.-B.; Song, H.-N.; Choi, J.-H.; Park, K.-H.; Woo, E.-J.
Deposited on : 2009-03-10
Resolution : 2.37 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

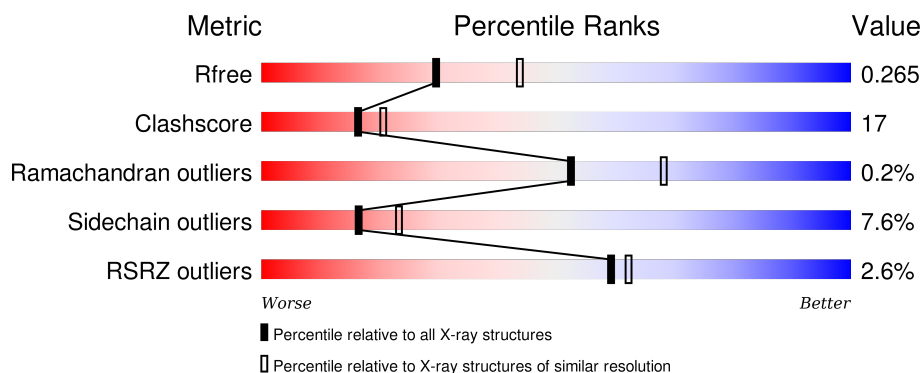
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

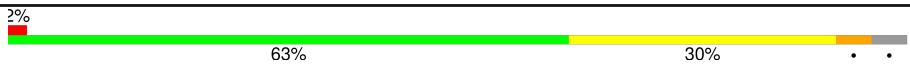
The reported resolution of this entry is 2.37 Å.

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}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3930 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	470	Total	C	N	O	S	0	0	1
			3790	2450	640	693	7			

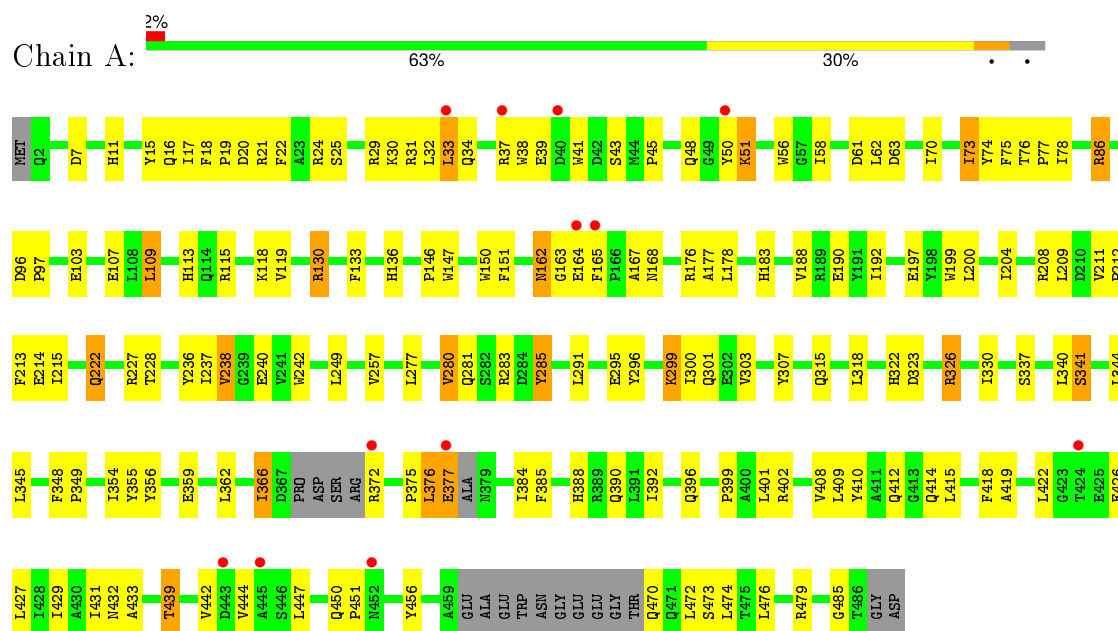
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	140	Total	O	0	0
			140	140		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	86.97Å 86.97Å 262.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.54 – 2.37 34.59 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.54-2.37) 99.1 (34.59-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 2.36Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.269 0.210 , 0.265	Depositor DCC
R_{free} test set	1190 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 24618 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3930	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/3903	0.57	0/5320

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	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	PHE	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	3790	0	3622	124	0
2	A	140	0	0	6	0
All	All	3930	0	3622	124	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 17.

All (124) 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:366:ILE:HD13	1:A:366:ILE:H	1.19	1.07
1:A:11:HIS:HD2	1:A:402:ARG:HE	1.06	0.95
1:A:32:LEU:HG	1:A:33:LEU:HD13	1.49	0.94
1:A:228:THR:HG21	1:A:237:ILE:HD11	1.47	0.93
1:A:73:ILE:HD11	1:A:119:VAL:HG22	1.56	0.87
1:A:11:HIS:CD2	1:A:402:ARG:HE	1.93	0.86
1:A:211:VAL:HG12	1:A:214:GLU:HG2	1.57	0.85
1:A:130:ARG:HD2	1:A:177:ALA:HA	1.63	0.80
1:A:76:THR:HB	1:A:77:PRO:HD2	1.69	0.73
1:A:366:ILE:H	1:A:366:ILE:CD1	2.00	0.73
1:A:43:SER:O	1:A:45:PRO:HD3	1.90	0.72
1:A:472:LEU:HD21	1:A:474:LEU:HB2	1.72	0.71
1:A:472:LEU:HD23	1:A:473:SER:N	2.06	0.70
1:A:50:TYR:O	1:A:51:LYS:N	2.25	0.69
1:A:299:LYS:HB3	1:A:299:LYS:NZ	2.08	0.69
1:A:76:THR:HB	1:A:77:PRO:CD	2.24	0.67
1:A:444:VAL:HG11	1:A:447:LEU:HD22	1.76	0.67
1:A:362:LEU:HD11	1:A:372:ARG:HH12	1.61	0.66
1:A:16:GLN:HG3	1:A:74:TYR:CE1	2.31	0.65
1:A:11:HIS:HD2	1:A:402:ARG:NE	1.89	0.65
1:A:211:VAL:HG13	1:A:213:PHE:CZ	2.31	0.65
1:A:20:ASP:OD1	1:A:86:ARG:HD2	1.98	0.64
1:A:211:VAL:CG1	1:A:214:GLU:HG2	2.27	0.64
1:A:322:HIS:HA	1:A:355:TYR:OH	1.98	0.63
1:A:301:GLN:NE2	1:A:408:VAL:HG21	2.14	0.62
1:A:418:PHE:CE1	1:A:429:ILE:HB	2.34	0.62
1:A:257:VAL:H	1:A:315:GLN:NE2	1.99	0.60
1:A:366:ILE:HD13	1:A:366:ILE:N	2.03	0.59
1:A:280:VAL:HG12	1:A:330:ILE:HD11	1.84	0.59
1:A:190:GLU:OE1	1:A:227:ARG:NH2	2.35	0.59
1:A:200:LEU:HD11	1:A:228:THR:HG23	1.84	0.59
1:A:15:TYR:HB2	1:A:70:ILE:HD12	1.85	0.59
1:A:301:GLN:HE21	1:A:408:VAL:HG21	1.68	0.59
1:A:73:ILE:HD13	1:A:73:ILE:H	1.69	0.58
1:A:472:LEU:HD23	1:A:472:LEU:C	2.26	0.56
1:A:162:ASN:HD22	1:A:164:GLU:H	1.53	0.56
1:A:73:ILE:HD13	1:A:118:LYS:O	2.04	0.56
1:A:295:GLU:O	1:A:299:LYS:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:CE2	1:A:48:GLN:HA	2.41	0.56
1:A:165:PHE:O	1:A:176:ARG:NH2	2.39	0.56
1:A:299:LYS:O	1:A:303:VAL:HG23	2.07	0.55
1:A:372:ARG:HG3	1:A:372:ARG:HH11	1.72	0.54
1:A:31:ARG:O	1:A:32:LEU:HB3	2.07	0.54
1:A:16:GLN:HG3	1:A:74:TYR:CZ	2.43	0.54
1:A:39:GLU:CD	1:A:39:GLU:H	2.11	0.54
1:A:211:VAL:O	1:A:211:VAL:HG12	2.07	0.53
1:A:183:HIS:CD2	1:A:215:ILE:HG13	2.43	0.53
1:A:63:ASP:OD2	1:A:115:ARG:NH2	2.41	0.53
1:A:439:THR:HA	1:A:474:LEU:O	2.09	0.53
1:A:197:GLU:OE1	1:A:227:ARG:HD3	2.08	0.53
1:A:133:PHE:O	1:A:136:HIS:HB3	2.09	0.52
1:A:344:LEU:HD21	1:A:431:ILE:HG13	1.91	0.52
1:A:472:LEU:CD2	1:A:474:LEU:HB2	2.39	0.52
1:A:103:GLU:O	1:A:107:GLU:HG3	2.10	0.52
1:A:209:LEU:O	1:A:212:PRO:HD3	2.12	0.50
1:A:37:ARG:HB3	1:A:39:GLU:OE1	2.11	0.50
1:A:22:PHE:HB3	2:A:2004:HOH:O	2.12	0.50
1:A:419:ALA:HA	1:A:427:LEU:O	2.11	0.49
1:A:240:GLU:HG2	2:A:2064:HOH:O	2.11	0.49
1:A:18:PHE:CD2	1:A:21:ARG:HB2	2.47	0.49
1:A:444:VAL:CG1	1:A:447:LEU:HD22	2.41	0.49
1:A:18:PHE:HD2	1:A:21:ARG:HB2	1.76	0.48
1:A:249:LEU:HD12	1:A:307:TYR:CE2	2.48	0.48
1:A:167:ALA:O	1:A:168:ASN:HB2	2.14	0.48
1:A:109:LEU:HD22	1:A:113:HIS:CE1	2.49	0.48
1:A:61:ASP:OD1	1:A:376:LEU:HD22	2.13	0.48
1:A:384:ILE:O	1:A:388:HIS:HD2	1.97	0.48
1:A:410:TYR:CZ	1:A:412:GLN:HB2	2.49	0.47
1:A:451:PRO:HB3	1:A:485:GLY:O	2.14	0.47
1:A:375:PRO:C	1:A:377:GLU:H	2.18	0.47
1:A:73:ILE:HG12	1:A:73:ILE:O	2.14	0.47
1:A:62:LEU:HD13	1:A:115:ARG:HD2	1.97	0.47
1:A:451:PRO:HA	1:A:485:GLY:O	2.14	0.47
1:A:30:LYS:HE3	1:A:38:TRP:CE2	2.49	0.47
1:A:163:GLY:HA2	1:A:176:ARG:CZ	2.45	0.46
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.79	0.46
1:A:291:LEU:CD1	1:A:299:LYS:HD2	2.46	0.46
1:A:354:ILE:CD1	1:A:392:ILE:HD11	2.44	0.46
1:A:211:VAL:HG12	1:A:214:GLU:CG	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TYR:N	1:A:285:TYR:CD2	2.84	0.46
1:A:73:ILE:CD1	1:A:119:VAL:HG22	2.36	0.46
1:A:479:ARG:HD3	2:A:2109:HOH:O	2.16	0.46
1:A:426:GLU:OE2	1:A:447:LEU:HA	2.16	0.45
1:A:30:LYS:HE3	1:A:38:TRP:CZ2	2.52	0.45
1:A:146:PRO:HG2	1:A:147:TRP:CE3	2.51	0.45
1:A:24:ARG:NE	1:A:51:LYS:O	2.50	0.45
1:A:283:ARG:NH2	1:A:323:ASP:OD2	2.49	0.45
1:A:281:GLN:HG2	1:A:323:ASP:OD1	2.17	0.44
1:A:396:GLN:HG3	2:A:2013:HOH:O	2.17	0.44
1:A:257:VAL:H	1:A:315:GLN:HE22	1.65	0.44
1:A:300:ILE:HD13	1:A:300:ILE:HA	1.83	0.44
1:A:299:LYS:HB3	1:A:299:LYS:HZ3	1.79	0.44
1:A:222:GLN:NE2	2:A:2069:HOH:O	2.50	0.44
1:A:222:GLN:NE2	1:A:222:GLN:H	2.16	0.43
1:A:291:LEU:HD13	1:A:299:LYS:HD2	2.00	0.43
1:A:25:SER:HB2	1:A:56:TRP:HB2	2.01	0.43
1:A:188:VAL:O	1:A:192:ILE:HG12	2.19	0.43
1:A:190:GLU:CD	1:A:227:ARG:HH22	2.21	0.43
1:A:450:GLN:HG2	1:A:470:GLN:HE22	1.84	0.43
1:A:356:TYR:O	1:A:356:TYR:CG	2.72	0.43
1:A:291:LEU:HD21	1:A:299:LYS:HE3	2.01	0.43
1:A:299:LYS:HB3	1:A:299:LYS:HZ2	1.84	0.43
1:A:109:LEU:HA	1:A:109:LEU:HD23	1.88	0.43
1:A:285:TYR:HD2	1:A:285:TYR:H	1.66	0.43
1:A:280:VAL:HG12	1:A:330:ILE:CD1	2.49	0.43
1:A:296:TYR:CZ	1:A:300:ILE:HG13	2.54	0.43
1:A:359:GLU:O	1:A:385:PHE:HA	2.18	0.43
1:A:76:THR:O	1:A:78:ILE:HG23	2.18	0.42
1:A:415:LEU:HD11	1:A:476:LEU:HD12	2.01	0.42
1:A:151:PHE:HB3	2:A:2050:HOH:O	2.18	0.42
1:A:199:TRP:HB3	1:A:204:ILE:HD13	2.00	0.42
1:A:280:VAL:CG2	1:A:280:VAL:O	2.67	0.42
1:A:337:SER:O	1:A:341:SER:HB2	2.21	0.41
1:A:96:ASP:HA	1:A:97:PRO:HD3	1.84	0.41
1:A:390:GLN:NE2	1:A:456:TYR:HD2	2.19	0.41
1:A:236:TYR:CE2	1:A:238:VAL:HG22	2.56	0.41
1:A:401:LEU:HG	1:A:427:LEU:CD1	2.52	0.40
1:A:348:PHE:CD1	1:A:349:PRO:HD2	2.56	0.40
1:A:22:PHE:CD1	1:A:58:ILE:HG12	2.56	0.40
1:A:414:GLN:HG3	1:A:433:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:O	1:A:19:PRO:HD3	2.21	0.40
1:A:147:TRP:O	1:A:150:TRP:HB2	2.22	0.40
1:A:236:TYR:CE2	1:A:238:VAL:CG2	3.04	0.40
1:A:399:PRO:HB2	1:A:422:LEU:HD23	2.02	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	459/488 (94%)	430 (94%)	28 (6%)	1 (0%)	52	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	LEU

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	393/409 (96%)	363 (92%)	30 (8%)	16	23

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	29	ARG
1	A	33	LEU
1	A	34	GLN
1	A	51	LYS
1	A	73	ILE
1	A	86	ARG
1	A	109	LEU
1	A	130	ARG
1	A	162	ASN
1	A	178	LEU
1	A	208	ARG
1	A	222	GLN
1	A	238	VAL
1	A	242	TRP
1	A	277	LEU
1	A	280	VAL
1	A	285	TYR
1	A	299	LYS
1	A	318	LEU
1	A	326	ARG
1	A	340	LEU
1	A	341	SER
1	A	345	LEU
1	A	366	ILE
1	A	377	GLU
1	A	409	LEU
1	A	432	ASN
1	A	439	THR
1	A	442	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	34	GLN
1	A	80	GLN
1	A	88	HIS
1	A	94	GLN
1	A	126	ASN
1	A	127	HIS
1	A	141	ASN
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	162	ASN
1	A	222	GLN
1	A	247	GLN
1	A	286	GLN
1	A	301	GLN
1	A	315	GLN
1	A	388	HIS
1	A	390	GLN
1	A	412	GLN
1	A	414	GLN
1	A	432	ASN
1	A	441	ASN
1	A	450	GLN
1	A	470	GLN
1	A	471	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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	470/488 (96%)	-0.17	12 (2%) 59 62	13, 24, 51, 71	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	THR	3.6
1	A	50	TYR	3.1
1	A	37	ARG	3.1
1	A	372	ARG	3.0
1	A	164	GLU	3.0
1	A	40	ASP	2.5
1	A	445	ALA	2.3
1	A	377	GLU	2.2
1	A	165	PHE	2.2
1	A	443	ASP	2.1
1	A	33	LEU	2.1
1	A	452	ASN	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 carbohydrates 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.