



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:47 PM UTC

PDB ID : 2DE0 / pdb\_00002de0  
Title : Crystal structure of human alpha 1,6-fucosyltransferase, FUT8  
Authors : Taniguchi, N.; Ihara, H.; Nakagawa, A.  
Deposited on : 2006-02-07  
Resolution : 2.61 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

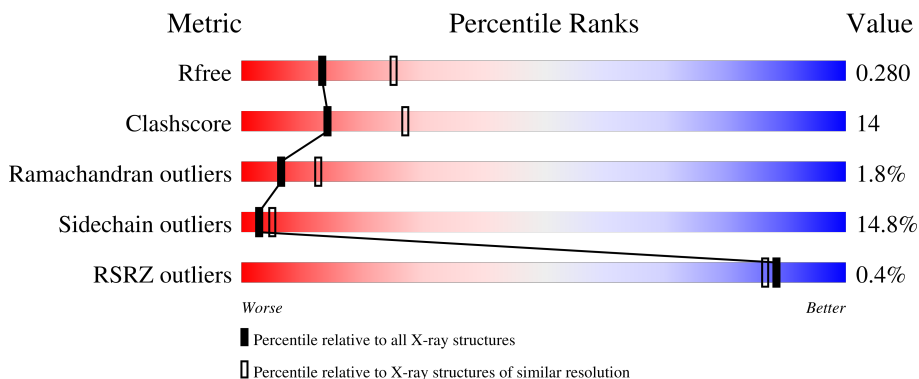
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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  $\geq 3$ , 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	X	526	 58% 21% 7% • 13%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3889 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-(1,6)-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	460	3752	2390	661	687	14	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	63	ALA	-	cloning artifact	UNP Q9BYC5
X	64	ASP	-	cloning artifact	UNP Q9BYC5
X	65	LEU	-	cloning artifact	UNP Q9BYC5
X	66	GLY	-	cloning artifact	UNP Q9BYC5
X	67	SER	-	cloning artifact	UNP Q9BYC5
X	576	ALA	-	expression tag	UNP Q9BYC5
X	577	GLY	-	expression tag	UNP Q9BYC5
X	578	GLY	-	expression tag	UNP Q9BYC5
X	579	GLY	-	expression tag	UNP Q9BYC5
X	580	HIS	-	expression tag	UNP Q9BYC5
X	581	HIS	-	expression tag	UNP Q9BYC5
X	582	HIS	-	expression tag	UNP Q9BYC5
X	583	HIS	-	expression tag	UNP Q9BYC5
X	584	HIS	-	expression tag	UNP Q9BYC5
X	585	HIS	-	expression tag	UNP Q9BYC5
X	586	GLY	-	expression tag	UNP Q9BYC5
X	587	GLY	-	expression tag	UNP Q9BYC5
X	588	GLY	-	expression tag	UNP Q9BYC5

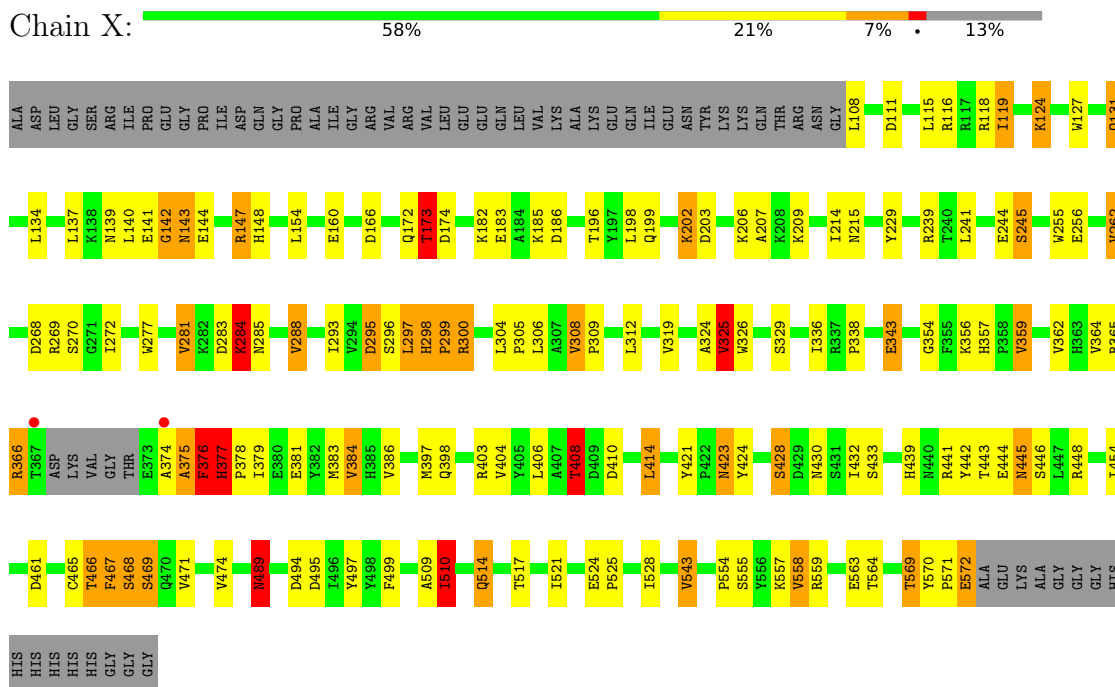
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	137	Total	O	0	0
			137	137		

### 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-(1,6)-fucosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.03Å 90.03Å 380.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.61 50.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.61) 97.9 (50.00-2.61)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.220 , 0.283 0.218 , 0.280	Depositor DCC
$R_{free}$ test set	1456 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtrriage
Anisotropy	0.561	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	X	0.97	4/3851 (0.1%)	1.15	17/5220 (0.3%)

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	X	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	119	ILE	CA-CB	6.62	1.62	1.54
1	X	384	VAL	CA-CB	6.10	1.61	1.54
1	X	474	VAL	CA-CB	5.72	1.61	1.54
1	X	300	ARG	N-CA	5.46	1.53	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	446	SER	N-CA-C	-7.12	103.85	112.54
1	X	543	VAL	CB-CA-C	-6.99	100.28	110.63
1	X	325	VAL	CB-CA-C	-6.90	101.08	112.26
1	X	514	GLN	CA-C-N	6.70	126.66	119.76
1	X	514	GLN	C-N-CA	6.70	126.66	119.76
1	X	173	THR	N-CA-C	6.04	123.67	110.80
1	X	510	ILE	CB-CA-C	5.93	118.36	111.55
1	X	468	SER	N-CA-C	-5.82	106.27	113.19
1	X	124	LYS	N-CA-C	-5.66	105.03	111.14
1	X	489	ASN	N-CA-C	5.50	118.81	112.97
1	X	408	THR	CB-CA-C	-5.50	97.34	109.56
1	X	521	ILE	CA-C-N	-5.41	115.01	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	521	ILE	C-N-CA	-5.41	115.01	120.31
1	X	445	ASN	N-CA-C	5.41	122.32	110.80
1	X	172	GLN	N-CA-C	5.38	120.51	113.30
1	X	428	SER	N-CA-C	5.30	117.31	108.99
1	X	270	SER	N-CA-C	5.21	116.65	110.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	298	HIS	Peptide
1	X	376	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	X	3752	0	3663	105	0
2	X	137	0	0	20	0
All	All	3889	0	3663	105	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 14.

All (105) 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:X:374:ALA:HA	2:X:705:HOH:O	1.51	1.11
1:X:365:ARG:HG3	2:X:624:HOH:O	1.59	1.01
1:X:423:ASN:HA	2:X:688:HOH:O	1.61	1.00
1:X:444:GLU:HG3	2:X:722:HOH:O	1.72	0.89
1:X:376:PHE:HA	1:X:381:GLU:OE2	1.75	0.86
1:X:439:HIS:HD2	1:X:442:TYR:HE1	1.24	0.85
1:X:124:LYS:HD2	2:X:598:HOH:O	1.81	0.80
1:X:510:ILE:HD13	1:X:559:ARG:CB	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:443:THR:OG1	1:X:445:ASN:ND2	2.14	0.79
1:X:572:GLU:HG2	2:X:717:HOH:O	1.82	0.79
1:X:510:ILE:HD13	1:X:559:ARG:HB3	1.64	0.78
1:X:569:THR:CG2	2:X:668:HOH:O	2.34	0.75
1:X:308:VAL:HG12	1:X:309:PRO:HD2	1.68	0.75
1:X:376:PHE:HA	1:X:381:GLU:CD	2.13	0.73
1:X:439:HIS:HD2	1:X:442:TYR:CE1	2.07	0.71
1:X:364:VAL:HB	1:X:408:THR:HG23	1.75	0.69
1:X:281:VAL:O	1:X:284:LYS:HB2	1.93	0.68
1:X:383:MET:HE2	1:X:386:VAL:HG21	1.77	0.65
1:X:137:LEU:CD2	1:X:148:HIS:HD2	2.10	0.65
1:X:433:SER:HA	1:X:448:ARG:NH1	2.13	0.63
1:X:465:CYS:SG	1:X:466:THR:N	2.72	0.63
1:X:377:HIS:CD2	2:X:619:HOH:O	2.51	0.63
1:X:375:ALA:HB1	2:X:700:HOH:O	1.98	0.63
1:X:199:GLN:NE2	1:X:262:VAL:HG13	2.15	0.62
1:X:111:ASP:HB2	1:X:173:THR:HG21	1.83	0.60
1:X:383:MET:CE	1:X:386:VAL:HG21	2.31	0.60
1:X:569:THR:HG23	2:X:668:HOH:O	2.00	0.60
1:X:377:HIS:HB3	1:X:378:PRO:HD3	1.82	0.60
1:X:137:LEU:HD23	1:X:148:HIS:HD2	1.67	0.59
1:X:199:GLN:HE21	1:X:262:VAL:HG13	1.67	0.59
1:X:338:PRO:HG2	1:X:343:GLU:HG3	1.84	0.58
1:X:244:GLU:HG3	1:X:269:ARG:HH12	1.69	0.57
1:X:365:ARG:NH2	2:X:706:HOH:O	2.38	0.57
1:X:127:TRP:O	1:X:131:GLN:HG2	2.05	0.57
1:X:141:GLU:O	1:X:142:GLY:C	2.47	0.57
1:X:509:ALA:HA	1:X:558:VAL:HG23	1.88	0.56
1:X:309:PRO:HG2	1:X:312:LEU:HD12	1.87	0.55
1:X:362:VAL:HG23	1:X:404:VAL:HG13	1.88	0.55
1:X:277:TRP:NE1	1:X:299:PRO:HG2	2.21	0.55
1:X:510:ILE:HD13	1:X:559:ARG:HB2	1.87	0.55
1:X:325:VAL:HG13	1:X:497:TYR:CZ	2.42	0.55
1:X:295:ASP:OD1	1:X:295:ASP:N	2.41	0.54
1:X:494:ASP:OD1	1:X:495:ASP:N	2.37	0.54
1:X:439:HIS:CD2	1:X:442:TYR:HE1	2.15	0.53
1:X:277:TRP:HE1	1:X:299:PRO:HG2	1.74	0.53
1:X:207:ALA:O	1:X:209:LYS:HG3	2.09	0.53
1:X:305:PRO:HG2	1:X:499:PHE:CD2	2.44	0.53
1:X:111:ASP:CB	1:X:173:THR:HG21	2.38	0.52
1:X:137:LEU:CD2	1:X:148:HIS:CD2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:142:GLY:O	1:X:143:ASN:C	2.53	0.52
1:X:554:PRO:HG2	1:X:557:LYS:HE3	1.90	0.52
1:X:174:ASP:OD1	2:X:724:HOH:O	2.19	0.52
1:X:147:ARG:HB2	1:X:147:ARG:NH1	2.25	0.51
1:X:202:LYS:NZ	1:X:202:LYS:HA	2.25	0.51
1:X:376:PHE:HA	1:X:381:GLU:OE1	2.09	0.51
1:X:461:ASP:O	1:X:489:ASN:ND2	2.43	0.51
1:X:443:THR:HG1	1:X:445:ASN:HD21	1.55	0.51
1:X:408:THR:HB	1:X:410:ASP:H	1.75	0.50
1:X:570:TYR:C	1:X:572:GLU:H	2.20	0.49
1:X:569:THR:HG22	2:X:668:HOH:O	2.05	0.49
1:X:139:ASN:O	1:X:140:LEU:HG	2.14	0.48
1:X:326:TRP:O	1:X:329:SER:OG	2.31	0.48
1:X:203:ASP:HB3	1:X:206:LYS:HG2	1.96	0.47
1:X:283:ASP:O	1:X:284:LYS:C	2.56	0.47
1:X:414:LEU:HD22	1:X:414:LEU:O	2.15	0.47
1:X:183:GLU:HA	1:X:183:GLU:OE1	2.15	0.46
1:X:306:LEU:HB3	1:X:324:ALA:HB1	1.97	0.46
1:X:357:HIS:HD2	1:X:461:ASP:OD2	1.98	0.46
1:X:359:VAL:HG13	1:X:403:ARG:HB3	1.96	0.46
1:X:467:PHE:C	1:X:469:SER:H	2.24	0.46
1:X:366:ARG:HD2	2:X:608:HOH:O	2.15	0.45
1:X:202:LYS:HA	1:X:202:LYS:HZ3	1.80	0.45
1:X:365:ARG:NH1	1:X:471:VAL:HG23	2.32	0.45
1:X:376:PHE:CA	1:X:381:GLU:OE1	2.64	0.45
1:X:444:GLU:O	2:X:722:HOH:O	2.21	0.44
1:X:376:PHE:N	1:X:376:PHE:CD1	2.86	0.44
1:X:308:VAL:O	1:X:564:THR:HA	2.18	0.43
1:X:277:TRP:CD1	1:X:297:LEU:HD21	2.53	0.43
1:X:300:ARG:NH2	1:X:304:LEU:HD13	2.33	0.43
1:X:209:LYS:O	1:X:239:ARG:HD3	2.19	0.43
1:X:283:ASP:O	1:X:285:ASN:N	2.51	0.42
1:X:524:GLU:O	1:X:525:PRO:C	2.59	0.42
1:X:466:THR:HG22	2:X:639:HOH:O	2.19	0.42
1:X:118:ARG:HD2	1:X:166:ASP:OD2	2.20	0.42
1:X:288:VAL:HG22	1:X:288:VAL:O	2.19	0.42
1:X:510:ILE:CD1	1:X:559:ARG:HE	2.32	0.42
1:X:559:ARG:NH2	2:X:687:HOH:O	2.51	0.42
1:X:467:PHE:C	1:X:469:SER:N	2.77	0.42
1:X:108:LEU:N	2:X:703:HOH:O	2.51	0.42
1:X:137:LEU:HG	1:X:148:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:572:GLU:CG	2:X:717:HOH:O	2.55	0.42
1:X:198:LEU:HD11	1:X:239:ARG:C	2.44	0.42
1:X:244:GLU:HG3	1:X:269:ARG:NH1	2.34	0.42
1:X:454:ILE:HG13	1:X:471:VAL:HG13	2.02	0.42
1:X:115:LEU:O	1:X:116:ARG:C	2.60	0.41
1:X:229:TYR:OH	1:X:297:LEU:HD12	2.20	0.41
1:X:308:VAL:HG23	1:X:563:GLU:O	2.19	0.41
1:X:293:ILE:HD12	1:X:295:ASP:CG	2.45	0.41
1:X:468:SER:HB3	1:X:495:ASP:OD1	2.21	0.41
1:X:245:SER:HB2	1:X:255:TRP:H	1.86	0.40
1:X:421:TYR:HB3	1:X:424:TYR:HD1	1.86	0.40
1:X:183:GLU:HG3	1:X:319:VAL:HG21	2.02	0.40
1:X:354:GLY:O	1:X:356:LYS:HB2	2.21	0.40
1:X:137:LEU:HA	1:X:140:LEU:HD12	2.04	0.40
1:X:570:TYR:HA	2:X:691:HOH:O	2.21	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	X	456/526 (87%)	408 (90%)	40 (9%)	8 (2%)	<b>6</b>   <b>13</b>

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	143	ASN
1	X	377	HIS
1	X	375	ALA
1	X	142	GLY
1	X	299	PRO
1	X	284	LYS

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Mol	Chain	Res	Type
1	X	571	PRO
1	X	298	HIS

### 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	X	405/454 (89%)	345 (85%)	60 (15%)	<b>3</b> <b>5</b>

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	119	ILE
1	X	131	GLN
1	X	134	LEU
1	X	144	GLU
1	X	147	ARG
1	X	154	LEU
1	X	160	GLU
1	X	173	THR
1	X	182	LYS
1	X	185	LYS
1	X	186	ASP
1	X	196	THR
1	X	202	LYS
1	X	214	ILE
1	X	215	ASN
1	X	241	LEU
1	X	245	SER
1	X	256	GLU
1	X	262	VAL
1	X	268	ASP
1	X	272	ILE
1	X	281	VAL
1	X	284	LYS
1	X	288	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	X	295	ASP
1	X	296	SER
1	X	297	LEU
1	X	308	VAL
1	X	325	VAL
1	X	336	ILE
1	X	343	GLU
1	X	359	VAL
1	X	366	ARG
1	X	376	PHE
1	X	377	HIS
1	X	379	ILE
1	X	384	VAL
1	X	397	MET
1	X	398	GLN
1	X	406	LEU
1	X	408	THR
1	X	414	LEU
1	X	423	ASN
1	X	428	SER
1	X	430	ASN
1	X	432	ILE
1	X	441	ARG
1	X	466	THR
1	X	467	PHE
1	X	469	SER
1	X	489	ASN
1	X	510	ILE
1	X	514	GLN
1	X	517	THR
1	X	528	ILE
1	X	543	VAL
1	X	555	SER
1	X	558	VAL
1	X	569	THR
1	X	572	GLU

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	X	148	HIS
1	X	226	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
1	X	285	ASN
1	X	357	HIS
1	X	439	HIS
1	X	445	ASN
1	X	489	ASN
1	X	491	HIS
1	X	514	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	460/526 (87%)	-0.19	2 (0%) 88 86	39, 61, 83, 91	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	374	ALA	3.4
1	X	367	THR	2.7

### 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.