



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:38 pm GMT

PDB ID : 2DE0
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

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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

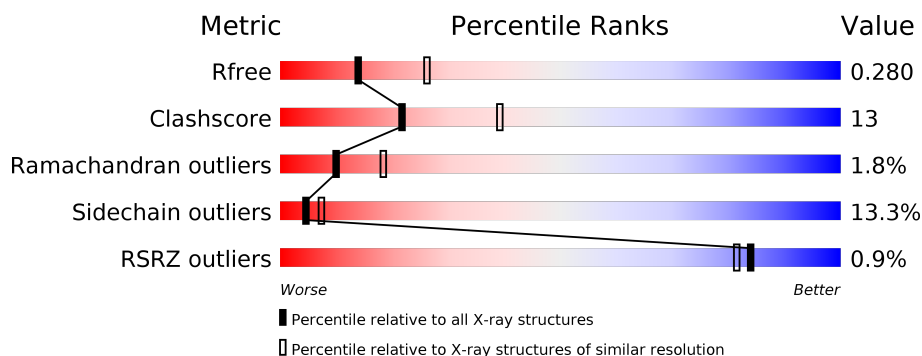
1 Overall quality at a glance

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}	100719	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (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 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	X	526	<div> <div></div> <div>61%19%6%13%</div> </div>

2 Entry composition

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
1	X	460	Total	C	N	O	S	0	0	0
			3752	2390	661	687	14			

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

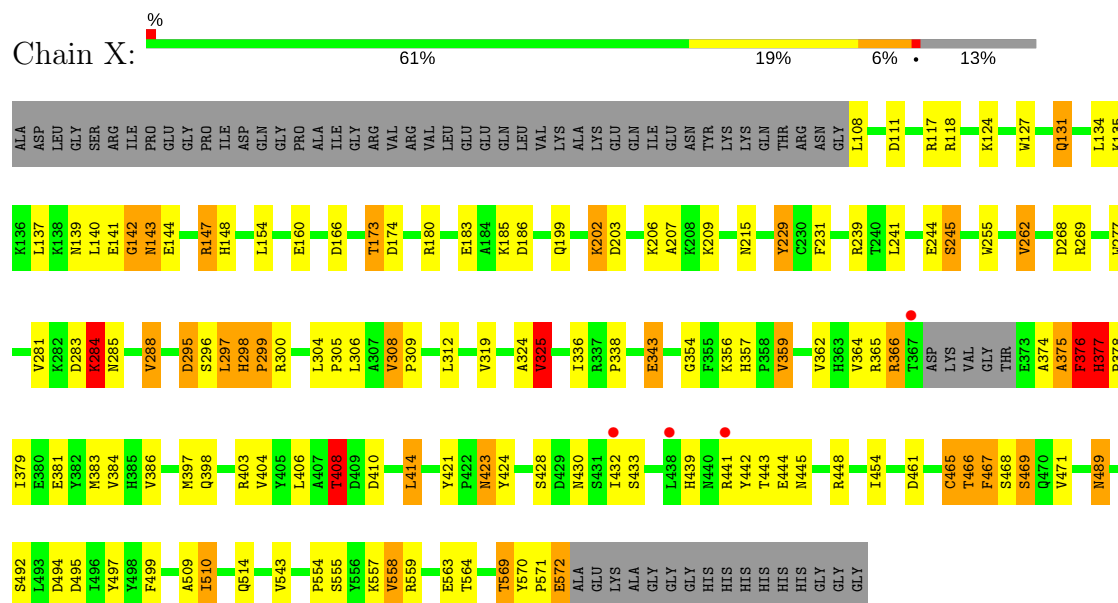
- Molecule 2 is water.

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 and DNA 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, α , β , γ	90.03Å 90.03Å 380.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.61 49.21 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.61) 97.6 (49.21-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.220 , 0.283 0.218 , 0.280	Depositor DCC
R_{free} test set	1448 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3889	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage'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.*

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	X	0.81	1/3851 (0.0%)	0.86	5/5220 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	465	CYS	CB-SG	-7.23	1.70	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	117	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	X	180	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	X	543	VAL	CB-CA-C	-5.85	100.28	111.40
1	X	325	VAL	CB-CA-C	-5.43	101.08	111.40
1	X	408	THR	CB-CA-C	-5.28	97.34	111.60

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 ⓘ

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	99	0
2	X	137	0	0	20	0
All	All	3889	0	3663	99	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 (99) 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
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: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:376:PHE:HA	1:X:381:GLU:CD	2.13	0.68
1:X:281:VAL:O	1:X:284:LYS:HB2	1.93	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:383:MET:HE2	1:X:386:VAL:HG21	1.85	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: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:141:GLU:O	1:X:142:GLY:C	2.47	0.52
1:X:137:LEU:CD2	1:X:148:HIS:CD2	2.92	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: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:142:GLY:O	1:X:143:ASN:C	2.53	0.47
1:X:203:ASP:HB3	1:X:206:LYS:HG2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:366:ARG:HD2	2:X:608:HOH:O	2.15	0.45
1:X:202:LYS:HZ3	1:X:202:LYS:HA	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:CD1	1:X:376:PHE:N	2.86	0.44
1:X:570:TYR:C	1:X:572:GLU:H	2.20	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:283:ASP:O	1:X:284:LYS:C	2.56	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:O	1:X:288:VAL:HG22	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: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
1:X:572:GLU:CG	2:X:717:HOH:O	2.55	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: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:467:PHE:C	1:X:469:SER:H	2.24	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

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	X	456/526 (87%)	408 (90%)	40 (9%)	8 (2%)	10	18

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
1	X	571	PRO
1	X	298	HIS

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	X	405/454 (89%)	351 (87%)	54 (13%)	4	7

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	131	GLN
1	X	134	LEU
1	X	135	LYS

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Mol	Chain	Res	Type
1	X	144	GLU
1	X	147	ARG
1	X	154	LEU
1	X	160	GLU
1	X	173	THR
1	X	185	LYS
1	X	186	ASP
1	X	202	LYS
1	X	215	ASN
1	X	229	TYR
1	X	231	PHE
1	X	241	LEU
1	X	245	SER
1	X	262	VAL
1	X	268	ASP
1	X	284	LYS
1	X	288	VAL
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

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Mol	Chain	Res	Type
1	X	469	SER
1	X	489	ASN
1	X	492	SER
1	X	510	ILE
1	X	514	GLN
1	X	555	SER
1	X	558	VAL
1	X	569	THR
1	X	572	GLU

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

Mol	Chain	Res	Type
1	X	146	GLN
1	X	148	HIS
1	X	226	HIS
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 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	X	460/526 (87%)	-0.08	4 (0%) 84 81	39, 61, 83, 91	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	432	ILE	4.5
1	X	367	THR	3.2
1	X	441	ARG	3.1
1	X	438	LEU	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.