



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 07:35 PM JST

PDB ID : 5XVM
Title : Sterol 3-beta-glucosyltransferase (ugt51) from *Saccharomyces cerevisiae*
(strain ATCC 204508 / S288c)
Authors : Feng, Y.; Chen, L.-Q.
Deposited on : 2017-06-28
Resolution : 2.77 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

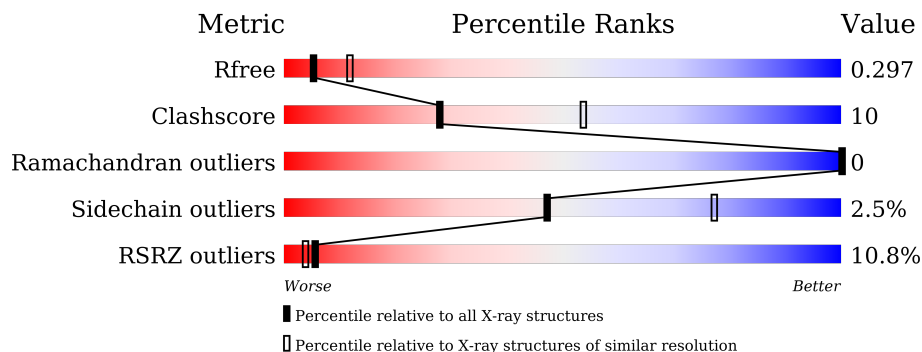
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	478	
1	B	478	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6441 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 Sterol 3-beta-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3253	2107	554	584	8	0	0	0
1	B	398	3163	2049	537	567	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	721	MET	-	expression tag	UNP Q06321
B	721	MET	-	expression tag	UNP Q06321

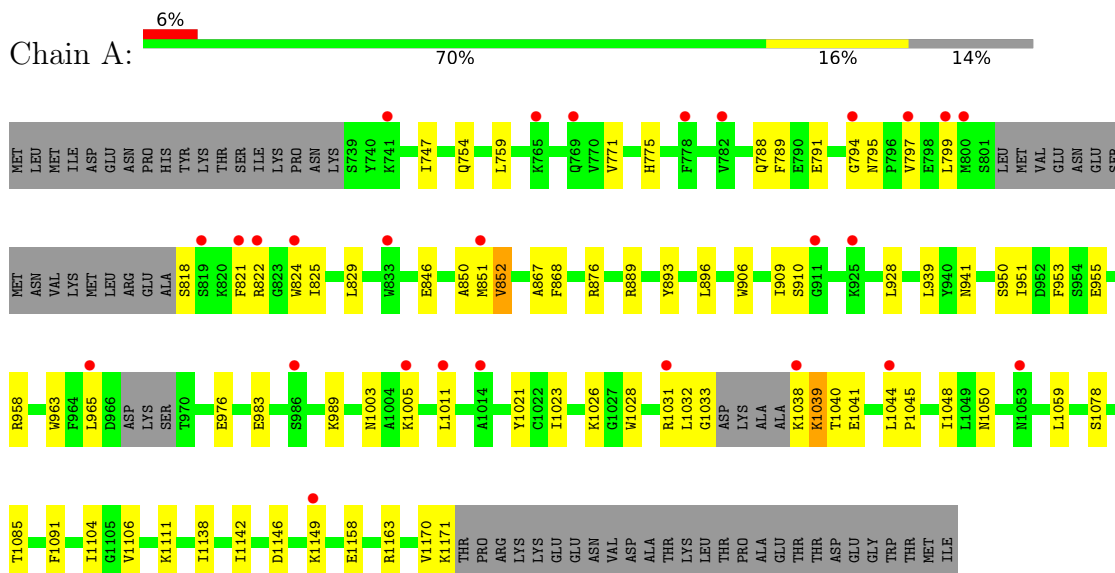
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	O	0	0
			11	11		
2	B	14	Total	O	0	0
			14	14		

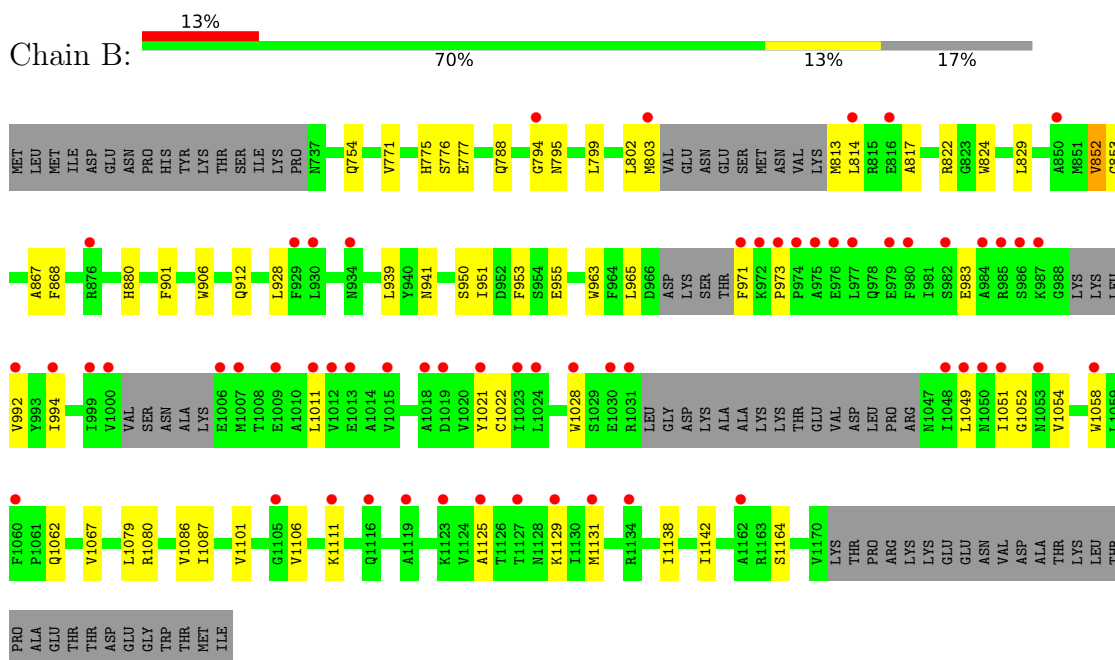
3 Residue-property plots [i](#)

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: Sterol 3-beta-glucosyltransferase



- Molecule 1: Sterol 3-beta-glucosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.86Å 83.57Å 151.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.01 – 2.77 51.01 – 2.77	Depositor EDS
% Data completeness (in resolution range)	86.6 (51.01-2.77) 86.6 (51.01-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.77Å)	Xtrriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.270 , 0.288 0.280 , 0.297	Depositor DCC
R_{free} test set	1989 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtrriage
Anisotropy	0.060	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6441	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	0.54	0/3331	0.78	3/4508 (0.1%)
1	B	0.54	0/3238	0.75	1/4380 (0.0%)
All	All	0.54	0/6569	0.76	4/8888 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1040	THR	N-CA-C	6.00	127.20	111.00
1	B	852	VAL	N-CA-C	5.72	126.43	111.00
1	A	852	VAL	N-CA-C	5.34	125.41	111.00
1	A	1163	ARG	NE-CZ-NH1	5.21	122.90	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3253	0	3275	87	0
1	B	3163	0	3164	59	0
2	A	11	0	0	1	0
2	B	14	0	0	0	0
All	All	6441	0	6439	127	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 10.

All (127) 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:893:TYR:CA	1:B:803:MET:HE1	1.39	1.52
1:A:893:TYR:HA	1:B:803:MET:CE	1.45	1.42
1:A:893:TYR:CA	1:B:803:MET:CE	1.98	1.39
1:A:1011:LEU:HD11	1:A:1028:TRP:CH2	1.66	1.30
1:A:1111:LYS:CG	1:B:1111:LYS:HD3	1.64	1.17
1:A:896:LEU:HD12	1:B:803:MET:SD	1.85	1.17
1:A:1038:LYS:HG2	1:A:1039:LYS:HE2	1.17	1.14
1:B:1011:LEU:HD11	1:B:1028:TRP:CH2	1.88	1.08
1:A:1111:LYS:HG3	1:B:1111:LYS:CD	1.84	1.06
1:A:893:TYR:N	1:B:803:MET:CE	2.17	1.06
1:B:1011:LEU:CD1	1:B:1028:TRP:CH2	2.40	1.03
1:A:1038:LYS:HG2	1:A:1039:LYS:CE	1.89	1.01
1:A:893:TYR:CA	1:B:803:MET:HE3	1.90	1.01
1:A:893:TYR:N	1:B:803:MET:HE3	1.72	1.00
1:A:876:ARG:HD2	2:A:1201:HOH:O	1.61	0.99
1:A:1011:LEU:CD1	1:A:1028:TRP:CH2	2.47	0.97
1:A:1011:LEU:HD11	1:A:1028:TRP:HH2	1.19	0.96
1:A:896:LEU:CD1	1:B:803:MET:SD	2.54	0.95
1:B:1011:LEU:CD1	1:B:1028:TRP:HH2	1.80	0.94
1:A:1011:LEU:CD1	1:A:1028:TRP:HH2	1.82	0.92
1:A:1078:SER:OG	1:A:1085:THR:HG21	1.73	0.87
1:A:1111:LYS:HG3	1:B:1111:LYS:HD3	0.88	0.83
1:B:1051:ILE:HD12	1:B:1051:ILE:O	1.80	0.82
1:A:893:TYR:CB	1:B:803:MET:CE	2.59	0.80
1:A:1011:LEU:HD11	1:A:1028:TRP:CZ2	2.17	0.80
1:A:1146:ASP:OD2	1:A:1149:LYS:HD2	1.85	0.76
1:A:1038:LYS:CG	1:A:1039:LYS:HE2	2.08	0.73
1:A:958:ARG:NH2	1:A:1158:GLU:OE2	2.24	0.70
1:A:1104:ILE:HG22	1:A:1106:VAL:HG13	1.75	0.68
1:A:1146:ASP:OD2	1:A:1149:LYS:CD	2.40	0.68
1:A:851:MET:CE	1:A:909:ILE:HG21	2.23	0.68
1:B:1067:VAL:HG22	1:B:1086:VAL:CG2	2.24	0.68
1:A:818:SER:O	1:A:822:ARG:HG3	1.93	0.68
1:A:893:TYR:CB	1:B:803:MET:HE3	2.22	0.67
1:A:983:GLU:OE2	1:A:1021:TYR:OH	2.10	0.67
1:A:1039:LYS:HE2	1:A:1039:LYS:N	2.10	0.66
1:A:1005:LYS:HG2	1:A:1041:GLU:HG2	1.78	0.66
1:A:1011:LEU:CD1	1:A:1028:TRP:CZ2	2.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:PHE:CZ	1:A:825:ILE:HD11	2.32	0.65
1:A:1044:LEU:HD11	1:A:1050:ASN:HB2	1.79	0.64
1:B:1011:LEU:CD1	1:B:1028:TRP:CZ2	2.80	0.64
1:A:893:TYR:H	1:B:803:MET:HE3	1.63	0.63
1:B:771:VAL:HG22	1:B:788:GLN:HB2	1.81	0.63
1:A:771:VAL:HG22	1:A:788:GLN:HB2	1.80	0.63
1:B:1049:LEU:HG	1:B:1051:ILE:HG23	1.80	0.63
1:B:1011:LEU:HD12	1:B:1028:TRP:CZ2	2.34	0.62
1:A:846:GLU:OE2	1:A:850:ALA:O	2.17	0.62
1:A:893:TYR:HB2	1:B:803:MET:HE3	1.80	0.61
1:A:893:TYR:HB2	1:B:803:MET:CE	2.30	0.61
1:B:1067:VAL:HG13	1:B:1086:VAL:HG23	1.84	0.60
1:A:794:GLY:HA2	1:A:824:TRP:CE2	2.37	0.59
1:A:1044:LEU:HD11	1:A:1050:ASN:CB	2.33	0.59
1:A:789:PHE:HE1	1:A:791:GLU:HG3	1.68	0.58
1:A:1044:LEU:CD1	1:A:1050:ASN:HB2	2.33	0.58
1:B:973:PRO:HG3	1:B:1058:TRP:CZ2	2.39	0.58
1:A:795:ASN:ND2	1:A:797:VAL:HG22	2.20	0.57
1:A:1038:LYS:CG	1:A:1039:LYS:CE	2.73	0.57
1:B:906:TRP:HB2	1:B:928:LEU:HD21	1.87	0.56
1:A:1031:ARG:HG2	1:A:1032:LEU:H	1.70	0.56
1:A:1031:ARG:NH2	1:A:1033:GLY:C	2.59	0.55
1:B:1067:VAL:HG22	1:B:1086:VAL:HG22	1.87	0.55
1:A:1031:ARG:HG2	1:A:1032:LEU:N	2.22	0.55
1:B:1087:ILE:HD12	1:B:1101:VAL:HG21	1.88	0.55
1:B:777:GLU:OE1	1:B:795:ASN:ND2	2.40	0.54
1:A:906:TRP:HB2	1:A:928:LEU:HD21	1.90	0.54
1:A:893:TYR:HA	1:B:803:MET:HE1	0.61	0.54
1:A:1038:LYS:HE2	1:A:1039:LYS:HE3	1.88	0.54
1:A:747:ILE:HG23	1:A:850:ALA:HB2	1.88	0.53
1:B:983:GLU:OE2	1:B:1021:TYR:OH	2.25	0.52
1:B:1106:VAL:HG11	1:B:1138:ILE:HG13	1.91	0.52
1:A:1111:LYS:CG	1:B:1111:LYS:CD	2.51	0.52
1:A:821:PHE:CE2	1:A:825:ILE:HD11	2.45	0.52
1:A:754:GLN:HG3	1:A:965:LEU:HD22	1.91	0.51
1:B:1051:ILE:HD12	1:B:1051:ILE:C	2.31	0.51
1:A:893:TYR:N	1:B:803:MET:HE1	1.98	0.49
1:B:754:GLN:HG3	1:B:965:LEU:HD22	1.93	0.49
1:B:1011:LEU:HD13	1:B:1028:TRP:HH2	1.74	0.49
1:B:802:LEU:HD22	1:B:817:ALA:HB1	1.95	0.48
1:A:794:GLY:O	1:A:824:TRP:CZ2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:829:LEU:HD23	1:B:852:VAL:HG12	1.95	0.47
1:A:795:ASN:CG	1:A:797:VAL:HG22	2.34	0.47
1:B:1080:ARG:HH11	1:B:1080:ARG:HG3	1.80	0.47
1:B:867:ALA:HA	1:B:939:LEU:O	2.15	0.47
1:B:1011:LEU:HD12	1:B:1028:TRP:CH2	2.38	0.46
1:A:1045:PRO:HD2	1:A:1048:ILE:HD12	1.96	0.46
1:A:1106:VAL:HG11	1:A:1138:ILE:HG13	1.97	0.46
1:A:1078:SER:CB	1:A:1085:THR:HG21	2.45	0.46
1:B:794:GLY:O	1:B:824:TRP:CZ2	2.69	0.46
1:B:880:HIS:CE1	1:B:901:PHE:CD2	3.05	0.45
1:A:1044:LEU:CD1	1:A:1050:ASN:CB	2.94	0.45
1:B:1125:ALA:HA	1:B:1131:MET:CE	2.46	0.45
1:A:1138:ILE:HG22	1:A:1142:ILE:HD12	1.98	0.45
1:B:852:VAL:HG23	1:B:853:GLY:N	2.32	0.44
1:A:851:MET:HE3	1:A:909:ILE:HG21	1.97	0.44
1:A:1170:VAL:O	1:A:1171:LYS:HB3	2.17	0.44
1:A:1146:ASP:OD2	1:A:1149:LYS:CE	2.65	0.44
1:A:989:LYS:HA	1:A:989:LYS:HD3	1.80	0.43
1:A:1038:LYS:HG2	1:A:1039:LYS:N	2.34	0.43
1:A:775:HIS:NE2	1:A:795:ASN:HA	2.33	0.43
1:A:1026:LYS:HE3	1:A:1041:GLU:OE1	2.18	0.43
1:A:1005:LYS:CG	1:A:1041:GLU:HG2	2.47	0.43
1:B:971:PHE:CZ	1:B:1054:VAL:HG13	2.54	0.43
1:A:789:PHE:HE1	1:A:791:GLU:CG	2.32	0.42
1:A:1031:ARG:CG	1:A:1032:LEU:H	2.31	0.42
1:A:794:GLY:C	1:A:824:TRP:CZ2	2.93	0.42
1:B:941:ASN:HB3	1:B:963:TRP:CE2	2.54	0.42
1:A:1011:LEU:HD12	1:A:1028:TRP:CZ2	2.55	0.42
1:A:1023:ILE:CD1	1:A:1059:LEU:HD11	2.50	0.42
1:B:950:SER:HB3	1:B:953:PHE:CD1	2.55	0.41
1:B:1051:ILE:HD13	1:B:1052:GLY:O	2.20	0.41
1:A:799:LEU:HD21	1:A:824:TRP:CD2	2.55	0.41
1:A:950:SER:HB3	1:A:953:PHE:CD1	2.55	0.41
1:B:822:ARG:HA	1:B:912:GLN:HE22	1.84	0.41
1:B:1138:ILE:HG22	1:B:1142:ILE:HD12	2.02	0.41
1:A:829:LEU:HD23	1:A:852:VAL:HG12	2.03	0.41
1:A:867:ALA:HA	1:A:939:LEU:O	2.20	0.41
1:B:775:HIS:NE2	1:B:795:ASN:HA	2.35	0.41
1:B:994:ILE:HD12	1:B:1022:CYS:SG	2.60	0.41
1:A:906:TRP:O	1:A:910:SER:N	2.54	0.41
1:B:1058:TRP:CH2	1:B:1062:GLN:OE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:794:GLY:O	1:B:824:TRP:HZ2	2.03	0.41
1:B:799:LEU:HD21	1:B:824:TRP:CD2	2.55	0.41
1:A:1038:LYS:HG2	1:A:1039:LYS:HE3	1.91	0.41
1:A:1146:ASP:OD2	1:A:1149:LYS:HE3	2.21	0.41
1:A:955:GLU:O	1:A:958:ARG:NH1	2.54	0.41
1:A:889:ARG:HD2	1:A:893:TYR:CE2	2.56	0.40
1:A:759:LEU:HD22	1:A:963:TRP:CZ3	2.56	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	402/478 (84%)	382 (95%)	20 (5%)	0	100	100
1	B	386/478 (81%)	366 (95%)	20 (5%)	0	100	100
All	All	788/956 (82%)	748 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	348/410 (85%)	341 (98%)	7 (2%)	55	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	337/410 (82%)	327 (97%)	10 (3%)	41	72
All	All	685/820 (84%)	668 (98%)	17 (2%)	47	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	868	PHE
1	A	941	ASN
1	A	951	ILE
1	A	976	GLU
1	A	1003	ASN
1	A	1039	LYS
1	A	1091	PHE
1	B	776	SER
1	B	813	MET
1	B	814	LEU
1	B	868	PHE
1	B	951	ILE
1	B	955	GLU
1	B	992	VAL
1	B	1079	LEU
1	B	1129	LYS
1	B	1164	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1003	ASN
1	B	892	ASN
1	B	927	ASN

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 monosaccharides 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	410/478 (85%)	0.58	27 (6%) 18 13	14, 26, 43, 65	0
1	B	398/478 (83%)	0.88	60 (15%) 2 1	13, 31, 49, 65	0
All	All	808/956 (84%)	0.73	87 (10%) 5 4	13, 28, 47, 65	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	975	ALA	7.9
1	A	794	GLY	5.5
1	B	986	SER	5.1
1	B	982	SER	5.1
1	B	972	LYS	4.7
1	A	822	ARG	4.7
1	B	973	PRO	4.5
1	B	803	MET	4.5
1	B	1049	LEU	4.4
1	B	980	PHE	4.1
1	A	821	PHE	4.0
1	B	1050	ASN	3.9
1	B	971	PHE	3.8
1	A	851	MET	3.8
1	B	985	ARG	3.6
1	A	800	MET	3.6
1	B	1021	TYR	3.5
1	B	1011	LEU	3.5
1	B	934	ASN	3.5
1	B	992	VAL	3.4
1	B	979	GLU	3.4
1	B	974	PRO	3.3
1	B	1028	TRP	3.3
1	B	929	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1031	ARG	3.2
1	B	1007	MET	3.1
1	A	1005	LYS	3.1
1	B	1125	ALA	3.1
1	B	1023	ILE	3.1
1	A	799	LEU	3.1
1	B	1129	LYS	3.0
1	B	1123	LYS	2.9
1	B	1105	GLY	2.9
1	B	1162	ALA	2.8
1	A	833	TRP	2.8
1	B	1060	PHE	2.8
1	B	1018	ALA	2.8
1	A	965	LEU	2.8
1	A	1031	ARG	2.8
1	B	1024	LEU	2.7
1	B	1058	TRP	2.6
1	A	1149	LYS	2.6
1	A	986	SER	2.6
1	B	1009	GLU	2.6
1	A	824	TRP	2.6
1	A	911	GLY	2.6
1	B	1019	ASP	2.5
1	B	1006	GLU	2.5
1	B	816	GLU	2.5
1	B	1116	GLN	2.5
1	B	984	ALA	2.5
1	B	1134	ARG	2.4
1	B	930	LEU	2.4
1	B	1013	GLU	2.4
1	A	1038	LYS	2.4
1	A	1014	ALA	2.4
1	A	819	SER	2.4
1	A	1044	LEU	2.4
1	B	976	GLU	2.3
1	A	782	VAL	2.3
1	B	1111	LYS	2.3
1	B	977	LEU	2.3
1	B	1127	THR	2.3
1	B	1051	ILE	2.3
1	B	850	ALA	2.2
1	A	741	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	876	ARG	2.2
1	B	1119	ALA	2.2
1	B	1048	ILE	2.2
1	B	1030	GLU	2.2
1	B	794	GLY	2.2
1	B	987	LYS	2.1
1	A	778	PHE	2.1
1	A	1053	ASN	2.1
1	B	814	LEU	2.1
1	B	1000	VAL	2.1
1	B	1012	VAL	2.1
1	B	1053	ASN	2.1
1	A	765	LYS	2.1
1	A	797	VAL	2.1
1	B	1015	VAL	2.1
1	A	925	LYS	2.1
1	A	1011	LEU	2.0
1	B	1131	MET	2.0
1	B	994	ILE	2.0
1	B	999	ILE	2.0
1	A	769	GLN	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 monosaccharides 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.