



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:28 PM GMT

PDB ID : 4RBN
Title : The crystal structure of Nitrosomonas europaea sucrose synthase: Insights into the evolutionary origin of sucrose metabolism in prokaryotes
Authors : Wu, R.; Asencion Diez, M.D.; Figueroa, C.M.; Machtey, M.; Iglesias, A.A.; Ballicora, M.A.; Liu, D.
Deposited on : 2014-09-12
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

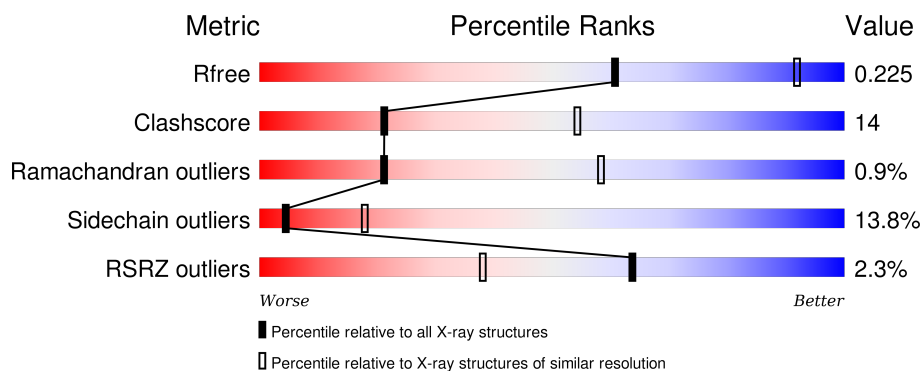
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	794	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 65%, yellow 65%, yellow 95%, orange 95%, orange 98%, red 98%, red 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 65% 29% 5% .. </div> </div>
1	B	794	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 64%, yellow 64%, yellow 94%, orange 94%, orange 97%, red 97%, red 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 64% 30% 6% . </div> </div>
1	C	794	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 65%, yellow 65%, yellow 93%, orange 93%, orange 96%, red 96%, red 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 2% 65% 28% 5% .. </div> </div>
1	D	794	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, green 6%, green 58%, yellow 58%, yellow 92%, orange 92%, orange 95%, red 95%, red 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 6% 58% 34% 7% .. </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25595 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 Sucrose synthase:Glycosyl transferases group 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	789	Total	C	N	O	S	0	0	0
			6332	4033	1106	1165	28			
1	C	789	Total	C	N	O	S	0	0	0
			6360	4047	1112	1173	28			
1	B	789	Total	C	N	O	S	0	0	0
			6346	4040	1106	1172	28			
1	D	789	Total	C	N	O	S	0	0	0
			6352	4039	1111	1174	28			

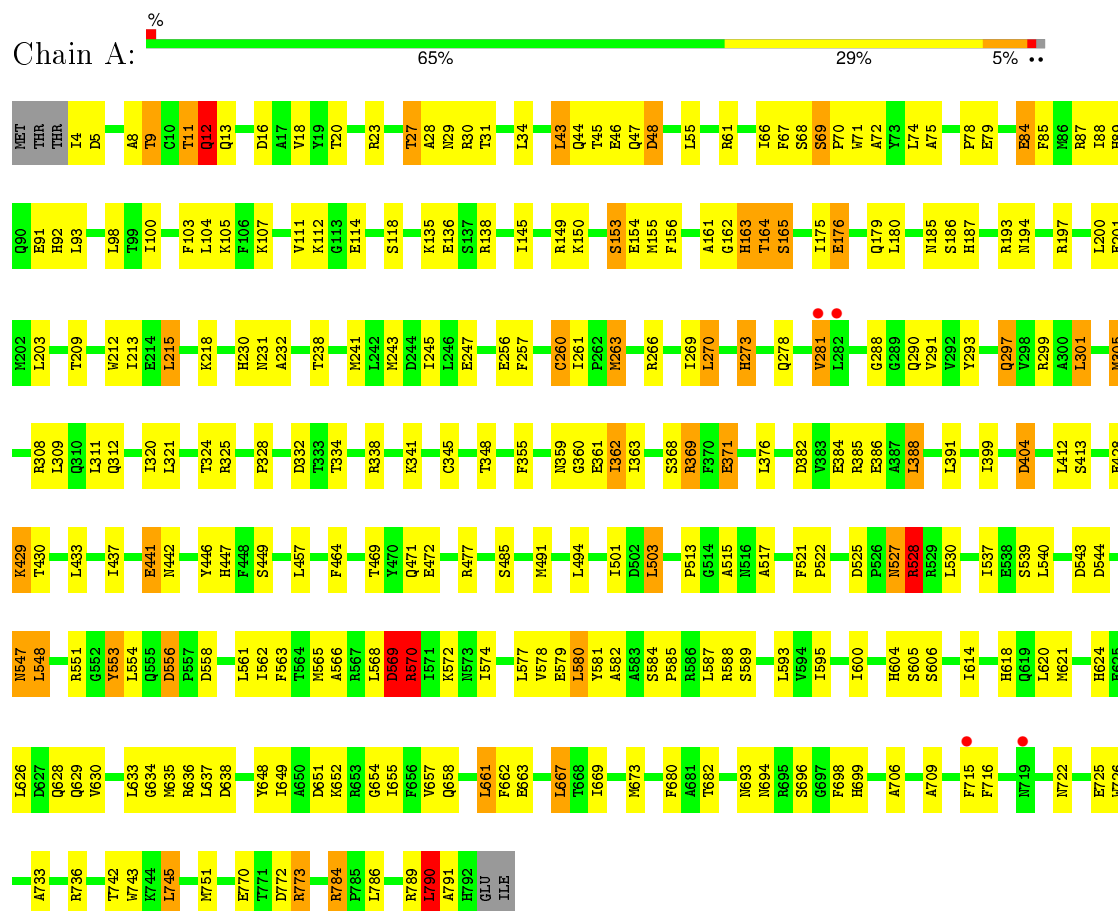
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	52	Total	O	0	0
			52	52		
2	C	50	Total	O	0	0
			50	50		
2	B	66	Total	O	0	0
			66	66		
2	D	37	Total	O	0	0
			37	37		

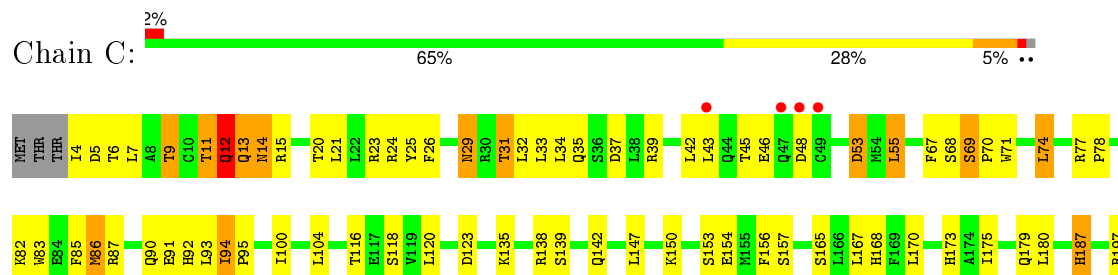
3 Residue-property plots

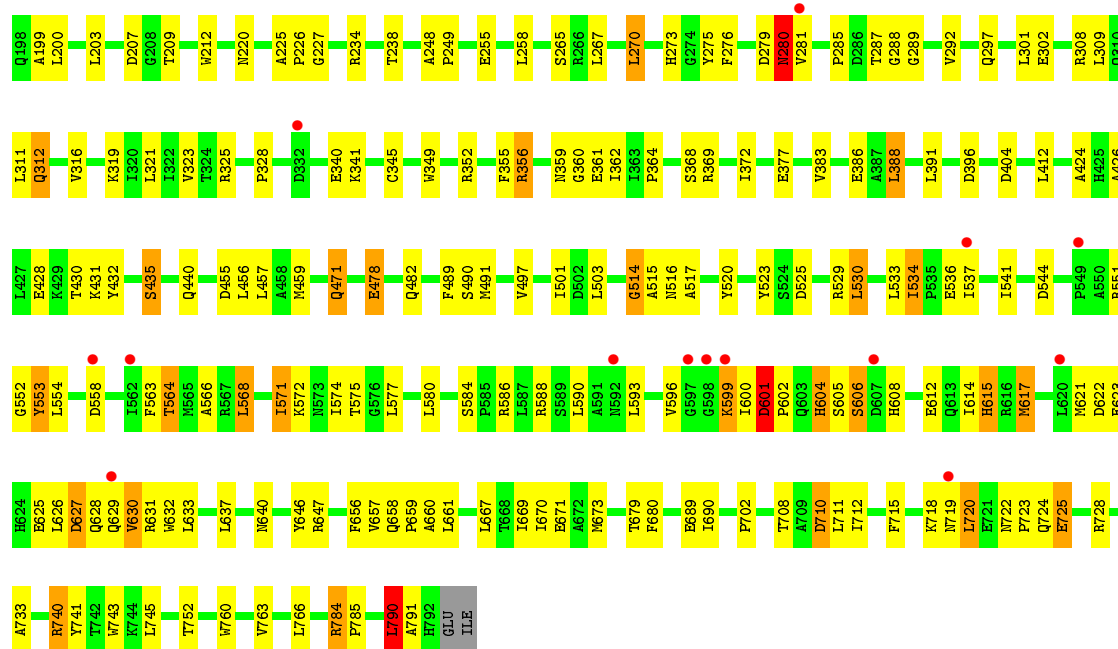
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Sucrose synthase:Glycosyl transferases group 1

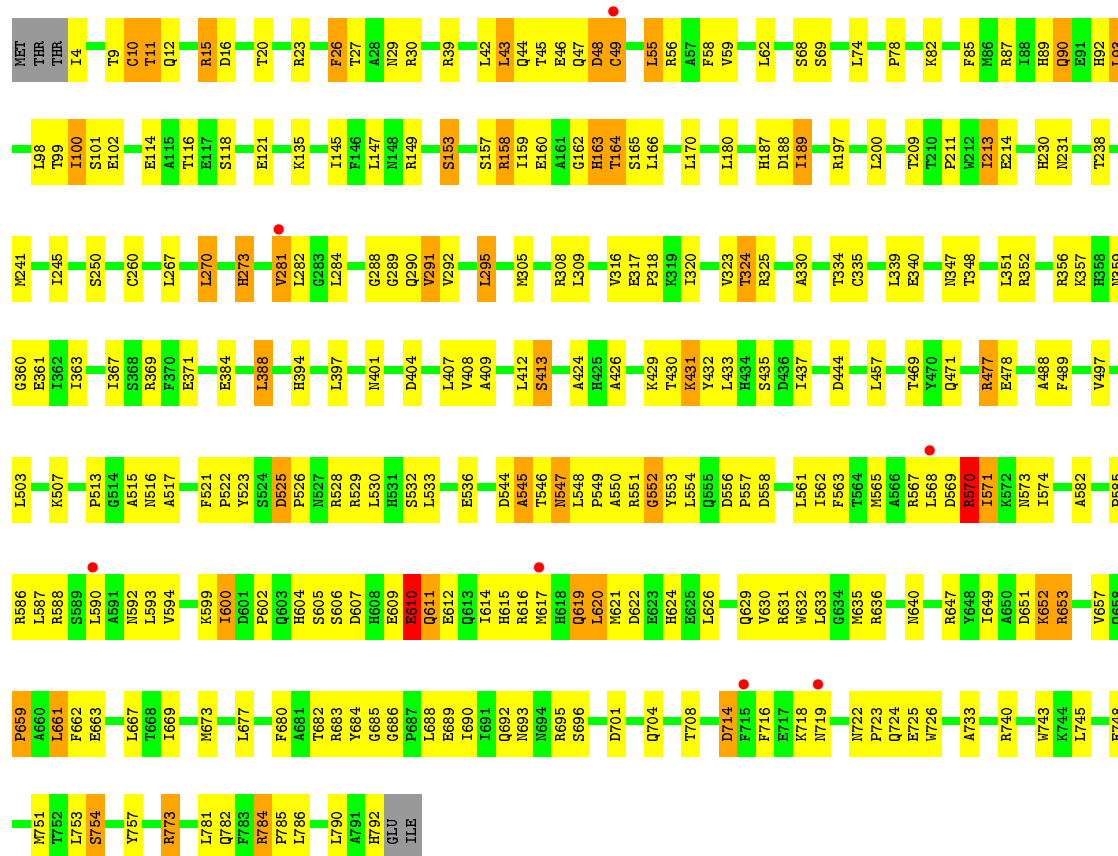


- Molecule 1: Sucrose synthase:Glycosyl transferases group 1

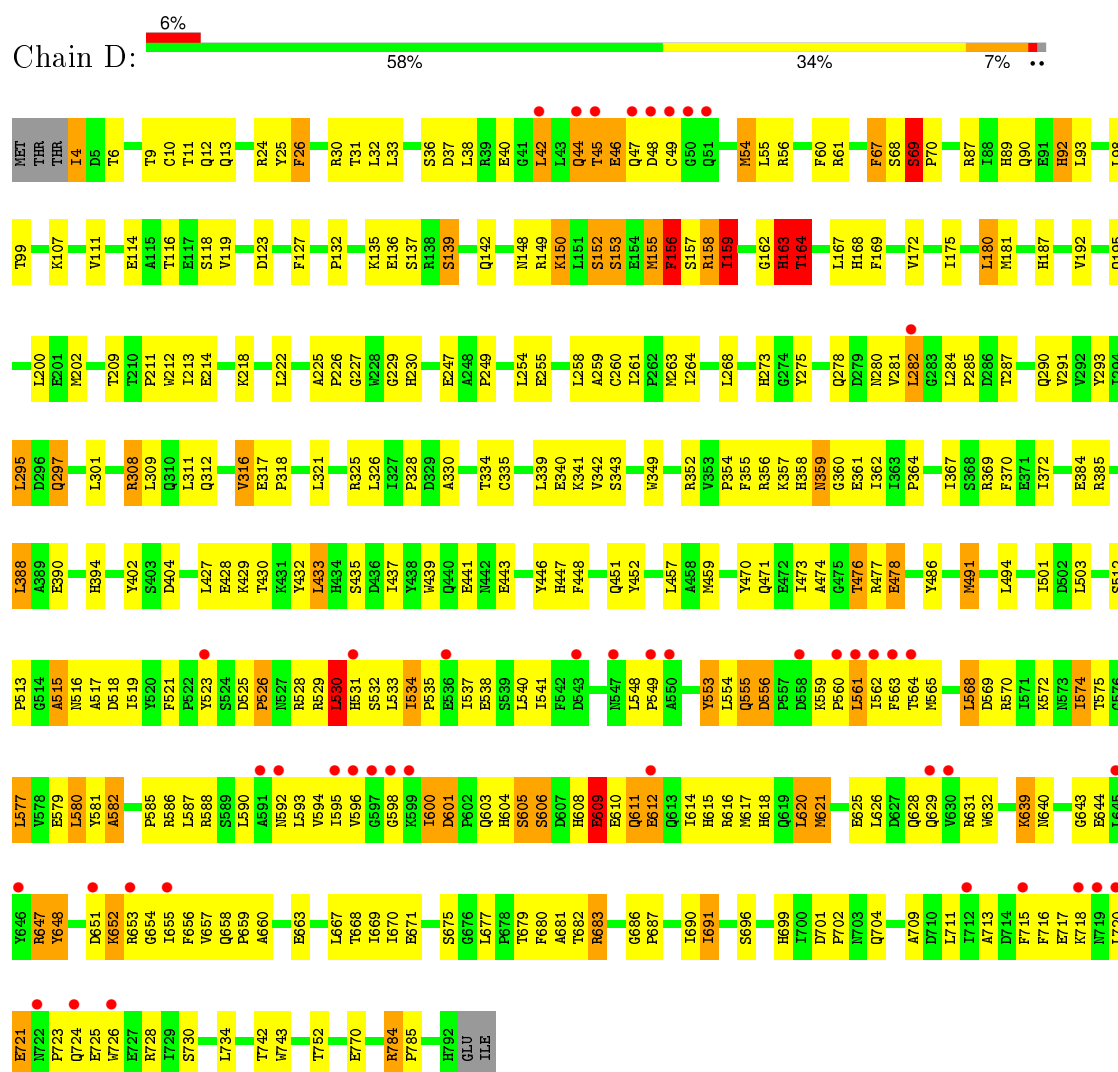




• Molecule 1: Sucrose synthase:Glycosyl transferases group 1



• Molecule 1: Sucrose synthase:Glycosyl transferases group 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	236.90Å 236.90Å 213.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.39 – 3.05 72.88 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (68.39-3.05) 93.5 (72.88-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.176 , 0.228 0.174 , 0.225	Depositor DCC
R_{free} test set	6051 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.0	EDS
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 126163 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25595	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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

5.1 Standard geometry

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	0.51	1/6481 (0.0%)	0.74	5/8786 (0.1%)
1	B	0.48	0/6496	0.73	0/8806
1	C	0.47	0/6511	0.70	1/8825 (0.0%)
1	D	0.46	0/6501	0.72	7/8812 (0.1%)
All	All	0.48	1/25989 (0.0%)	0.72	13/35229 (0.0%)

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	6
1	B	0	5
1	C	0	6
1	D	0	12
All	All	0	29

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	CYS	CB-SG	-7.03	1.70	1.82

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	530	LEU	CA-CB-CG	6.82	130.98	115.30
1	D	163	HIS	N-CA-C	-6.72	92.86	111.00
1	D	611	GLN	N-CA-C	-6.63	93.10	111.00
1	A	790	LEU	N-CA-C	6.37	128.19	111.00
1	A	569	ASP	C-N-CA	6.26	137.35	121.70

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLN	Peptide
1	A	13	GLN	Peptide
1	A	27	THR	Peptide
1	A	359	ASN	Peptide
1	A	551	ARG	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	A	6332	0	6210	169	0
1	B	6346	0	6220	177	0
1	C	6360	0	6240	167	0
1	D	6352	0	6235	218	0
2	A	52	0	0	1	0
2	B	66	0	0	4	0
2	C	50	0	0	0	0
2	D	37	0	0	0	0
All	All	25595	0	24905	716	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.

The worst 5 of 716 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:D:516:ASN:HB3	1:D:518:ASP:H	1.25	1.01
1:D:654:GLY:O	1:D:655:ILE:HD13	1.66	0.94
1:D:360:GLY:HA2	1:D:361:GLU:HB3	1.52	0.91
1:D:654:GLY:O	1:D:655:ILE:CD1	2.22	0.86
1:D:369:ARG:NH2	1:D:428:GLU:OE2	2.08	0.86

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	A	787/794 (99%)	707 (90%)	78 (10%)	2 (0%)	46	78
1	B	787/794 (99%)	699 (89%)	76 (10%)	12 (2%)	13	44
1	C	787/794 (99%)	713 (91%)	68 (9%)	6 (1%)	24	61
1	D	787/794 (99%)	692 (88%)	88 (11%)	7 (1%)	21	58
All	All	3148/3176 (99%)	2811 (89%)	310 (10%)	27 (1%)	21	58

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	ASN
1	B	160	GLU
1	B	189	ILE
1	C	11	THR
1	B	11	THR

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	A	673/687 (98%)	576 (86%)	97 (14%)	4	16
1	B	677/687 (98%)	583 (86%)	94 (14%)	4	18
1	C	680/687 (99%)	598 (88%)	82 (12%)	6	23
1	D	679/687 (99%)	579 (85%)	100 (15%)	4	15
All	All	2709/2748 (99%)	2336 (86%)	373 (14%)	4	18

5 of 373 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	640	ASN
1	B	273	HIS
1	D	575	THR
1	C	725	GLU
1	B	48	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	290	GLN
1	C	719	ASN
1	D	92	HIS
1	A	401	ASN
1	B	719	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 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 ⓘ

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	789/794 (99%)	-0.36	4 (0%) 91 81	8, 37, 104, 170	0
1	B	789/794 (99%)	-0.33	7 (0%) 85 69	9, 38, 103, 152	0
1	C	789/794 (99%)	-0.16	18 (2%) 64 38	10, 46, 111, 167	0
1	D	789/794 (99%)	0.01	45 (5%) 27 11	11, 60, 140, 180	0
All	All	3156/3176 (99%)	-0.21	74 (2%) 64 38	8, 44, 116, 180	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	562	ILE	5.8
1	A	281	VAL	5.4
1	A	282	LEU	5.4
1	D	49	CYS	4.8
1	C	719	ASN	4.4

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.