



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 07:44 PM BST

PDB ID : 5X2O  
Title : Crystal structure of the medaka fish taste receptor T1r2a-T1r3 ligand binding domains in complex with L-arginine  
Authors : Nuemket, N.; Yasui, N.; Atsumi, N.; Yamashita, A.  
Deposited on : 2017-02-02  
Resolution : 2.60 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](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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

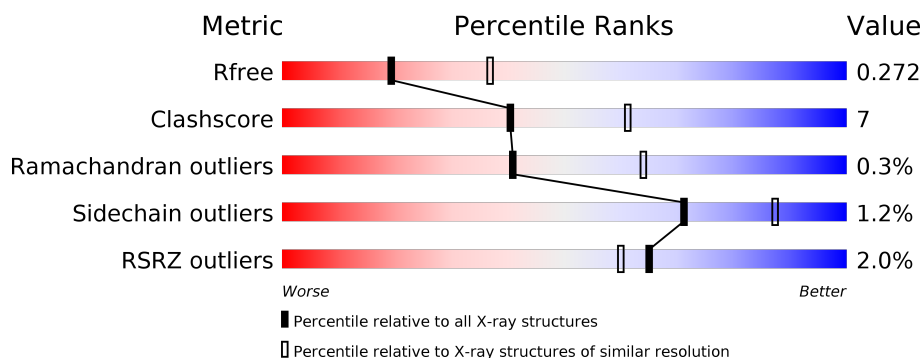
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	A	461	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>9%</div> </div> </div>
1	C	461	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
2	B	478	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• 5%</div> </div> </div>
2	D	478	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>8%</div> </div> </div>
3	H	225	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>•</div> </div> </div>
3	J	225	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	K	217	
4	L	217	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	902	-	-	-	X
5	NAG	B	901	-	-	-	X
5	NAG	B	905	-	-	-	X
5	NAG	D	904	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21165 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 Taste receptor, type 1, member 2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3338	2159	551	611	17			
1	C	426	Total	C	N	O	S	0	1	0
			3370	2174	558	621	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	SER	-	expression tag	UNP A0A173M0G2
A	476	GLY	-	expression tag	UNP A0A173M0G2
A	477	ILE	-	expression tag	UNP A0A173M0G2
A	478	GLU	-	expression tag	UNP A0A173M0G2
A	479	GLY	-	expression tag	UNP A0A173M0G2
A	480	ARG	-	expression tag	UNP A0A173M0G2
C	475	SER	-	expression tag	UNP A0A173M0G2
C	476	GLY	-	expression tag	UNP A0A173M0G2
C	477	ILE	-	expression tag	UNP A0A173M0G2
C	478	GLU	-	expression tag	UNP A0A173M0G2
C	479	GLY	-	expression tag	UNP A0A173M0G2
C	480	ARG	-	expression tag	UNP A0A173M0G2

- Molecule 2 is a protein called Taste receptor, type 1, member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	452	Total	C	N	O	S	0	0	0
			3540	2274	569	682	15			
2	D	441	Total	C	N	O	S	0	0	0
			3451	2221	557	658	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	492	SER	-	expression tag	UNP A0A173M094
B	493	GLY	-	expression tag	UNP A0A173M094
B	494	ILE	-	expression tag	UNP A0A173M094
B	495	GLU	-	expression tag	UNP A0A173M094
B	496	GLY	-	expression tag	UNP A0A173M094
B	497	ARG	-	expression tag	UNP A0A173M094
D	492	SER	-	expression tag	UNP A0A173M094
D	493	GLY	-	expression tag	UNP A0A173M094
D	494	ILE	-	expression tag	UNP A0A173M094
D	495	GLU	-	expression tag	UNP A0A173M094
D	496	GLY	-	expression tag	UNP A0A173M094
D	497	ARG	-	expression tag	UNP A0A173M094

- Molecule 3 is a protein called Fab16A Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1662	1056	274	324	8			
3	J	220	Total	C	N	O	S	0	0	0
			1665	1057	274	326	8			

- Molecule 4 is a protein called Fab16A Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	216	Total	C	N	O	S	0	0	0
			1670	1035	287	342	6			
4	K	216	Total	C	N	O	S	0	0	0
			1670	1035	287	342	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



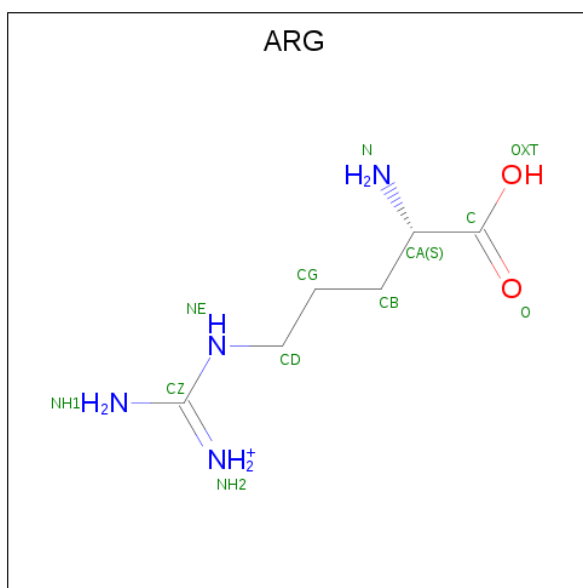
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	4	2		
6	B	1	Total	C	N	O	0	1
			20	11	7	2		
6	C	1	Total	C	N	O	0	0
			12	6	4	2		
6	D	1	Total	C	N	O	0	1
			20	11	7	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Na	0	0
			2	2		
7	D	1	Total	Na	0	0
			1	1		
7	C	2	Total	Na	0	0
			2	2		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	K	1	Total	Ca	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	73	Total	O	0	0
			73	73		
10	B	48	Total	O	0	0
			48	48		
10	C	71	Total	O	0	0
			71	71		

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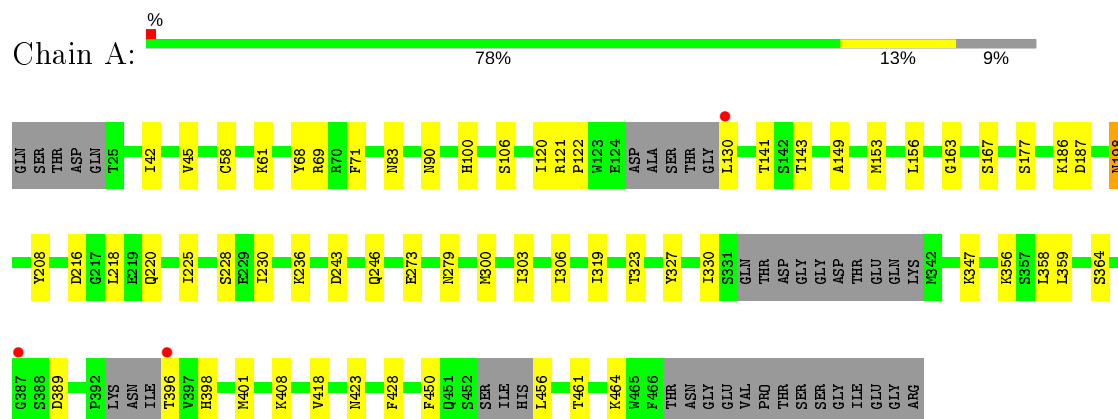
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	43	Total 43	O 43	0	0
10	H	39	Total 39	O 39	0	0
10	L	34	Total 34	O 34	0	0
10	J	31	Total 31	O 31	0	0
10	K	24	Total 24	O 24	0	0

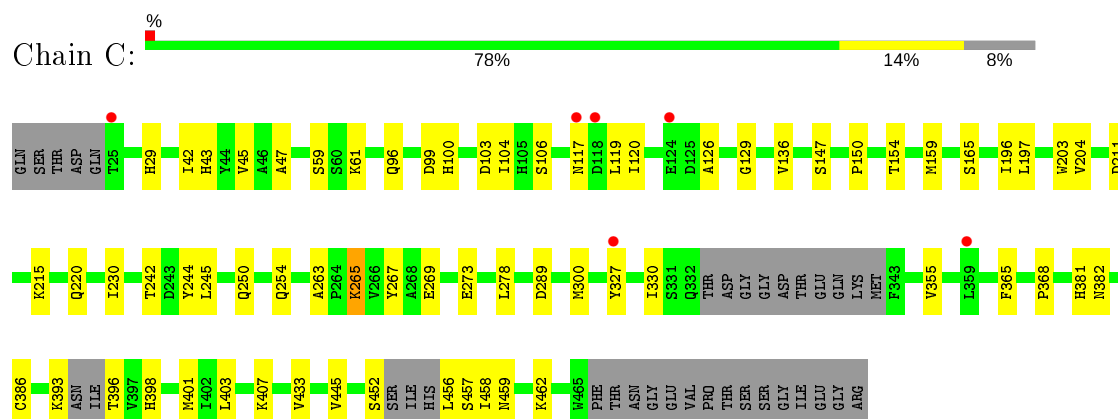
### 3 Residue-property plots

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.

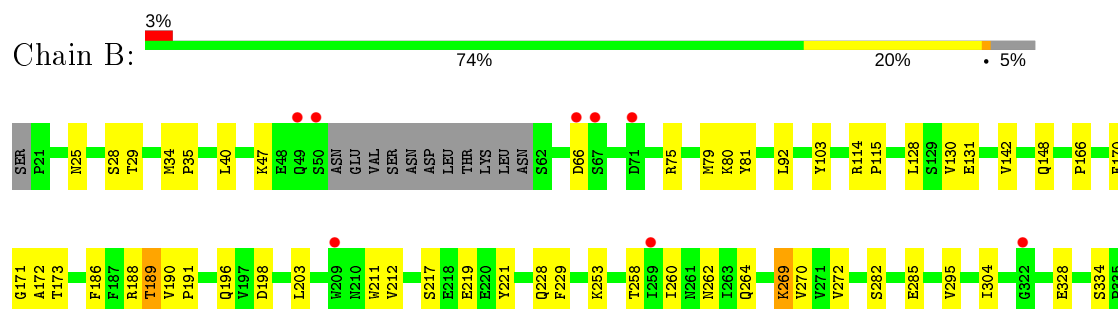
- Molecule 1: Taste receptor, type 1, member 2a

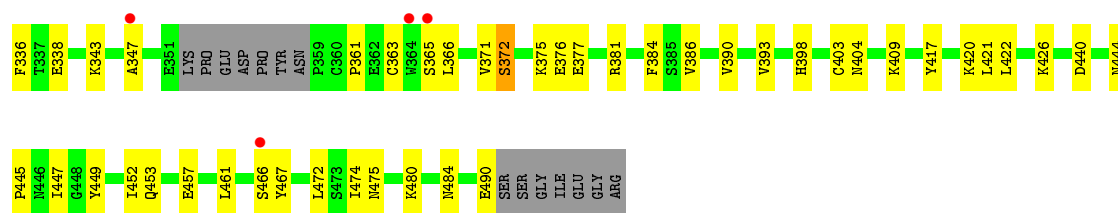


- Molecule 1: Taste receptor, type 1, member 2a

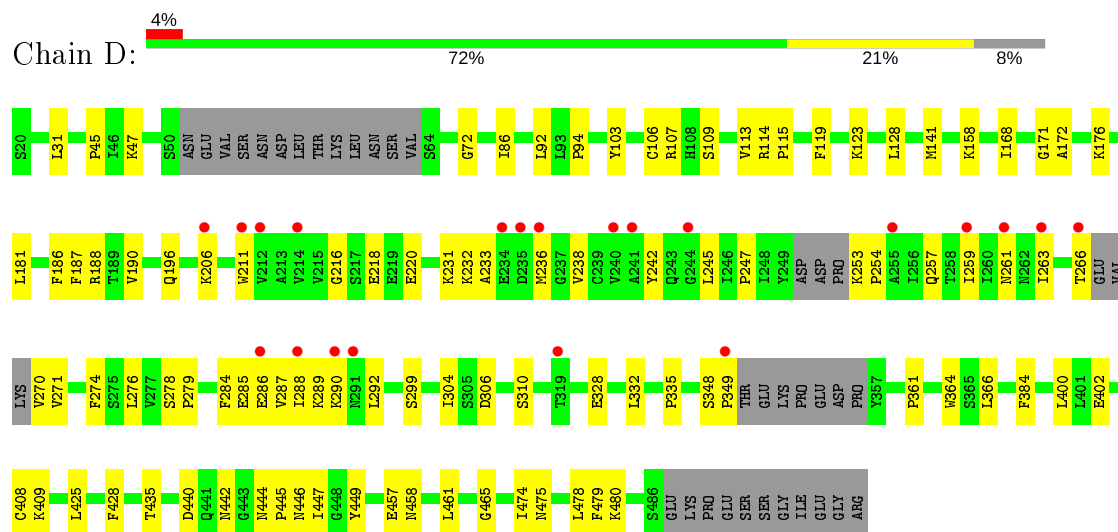


- Molecule 2: Taste receptor, type 1, member 3

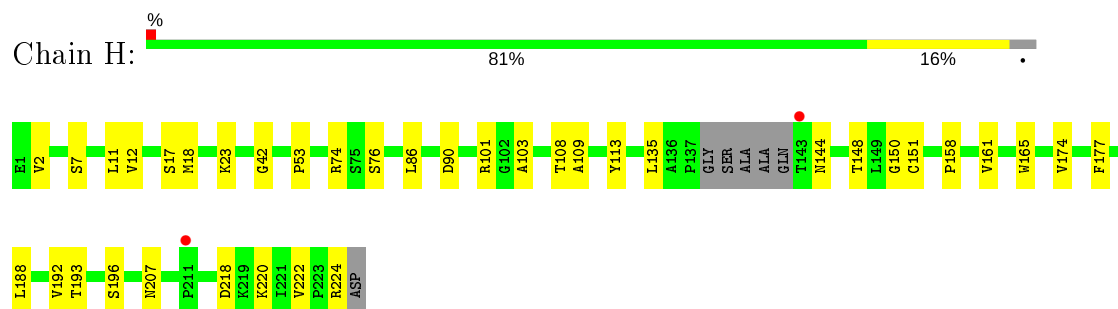




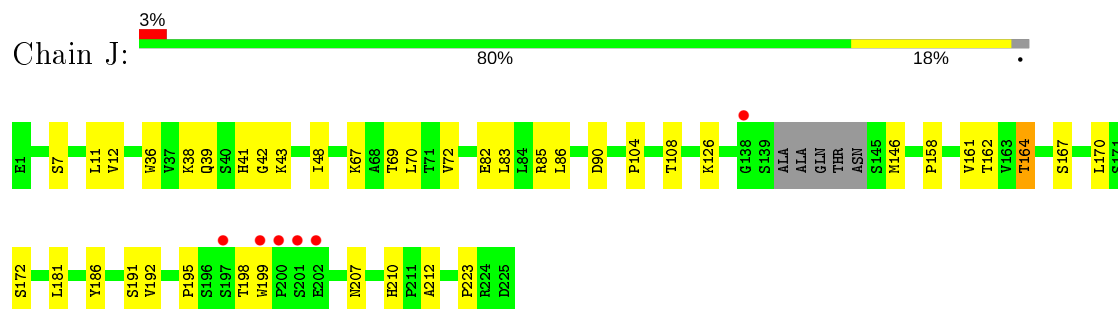
• Molecule 2: Taste receptor, type 1, member 3



• Molecule 3: Fab16A Heavy chain



• Molecule 3: Fab16A Heavy chain

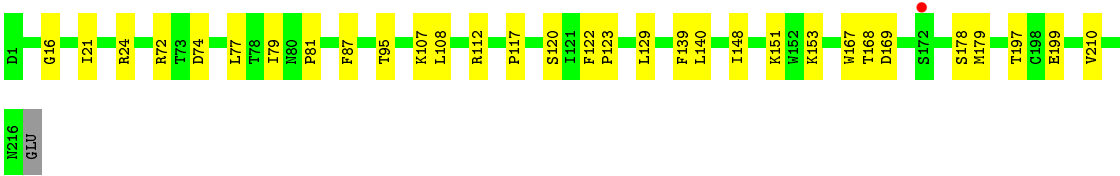
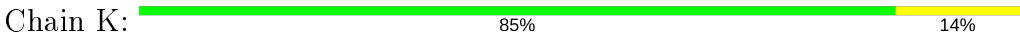


• Molecule 4: Fab16A Light chain





● Molecule 4: Fab16A Light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.91Å 113.68Å 128.64Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	49.41 – 2.60 49.42 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.5 (49.41-2.60) 95.5 (49.42-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.185 , 0.272 0.186 , 0.272	Depositor DCC
$R_{free}$ test set	4231 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, NAG, CL

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	0.45	0/3423	0.58	0/4646
1	C	0.48	0/3458	0.59	0/4695
2	B	0.42	0/3621	0.56	1/4923 (0.0%)
2	D	0.41	0/3529	0.56	0/4797
3	H	0.42	0/1706	0.58	0/2331
3	J	0.44	0/1709	0.60	0/2334
4	K	0.46	0/1707	0.60	0/2320
4	L	0.44	0/1707	0.61	0/2320
All	All	0.44	0/20860	0.58	1/28366 (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
2	D	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	490	GLU	OE1-CD-OE2	-5.33	116.90	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	289	LYS	Peptide
3	J	42	GLY	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	3338	0	3258	38	0
1	C	3370	0	3290	46	0
2	B	3540	0	3495	64	0
2	D	3451	0	3409	75	0
3	H	1662	0	1642	24	0
3	J	1665	0	1641	24	1
4	K	1670	0	1596	19	0
4	L	1670	0	1596	12	0
5	A	98	0	91	2	0
5	B	98	0	91	2	1
5	C	112	0	104	1	0
5	D	56	0	52	1	0
6	A	12	0	12	1	0
6	B	20	0	24	2	0
6	C	12	0	12	1	0
6	D	20	0	24	6	0
7	A	2	0	0	0	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
8	B	1	0	0	1	0
8	D	1	0	0	0	0
9	K	1	0	0	0	0
10	A	73	0	0	5	0
10	B	48	0	0	5	0
10	C	71	0	0	2	0
10	D	43	0	0	5	0
10	H	39	0	0	1	0
10	J	31	0	0	2	0
10	K	24	0	0	1	0
10	L	34	0	0	0	0
All	All	21165	0	20337	294	1

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 7.

The worst 5 of 294 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:423:ASN:O	10:A:1001:HOH:O	1.92	0.87
2:D:276:LEU:HD22	6:D:951[A]:ARG:HD2	1.57	0.84
1:C:398:HIS:H	1:C:401:MET:HE2	1.39	0.83
2:D:253:LYS:N	10:D:602:HOH:O	2.17	0.78
1:A:408:LYS:NZ	10:A:1002:HOH:O	2.18	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:72:VAL:O	5:B:906:NAG:O4[2_755]	2.11	0.09

## 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	411/461 (89%)	389 (95%)	20 (5%)	2 (0%)	29	52
1	C	419/461 (91%)	399 (95%)	19 (4%)	1 (0%)	47	71
2	B	446/478 (93%)	420 (94%)	25 (6%)	1 (0%)	47	71
2	D	431/478 (90%)	404 (94%)	26 (6%)	1 (0%)	47	71
3	H	215/225 (96%)	209 (97%)	6 (3%)	0	100	100
3	J	216/225 (96%)	209 (97%)	7 (3%)	0	100	100
4	K	214/217 (99%)	208 (97%)	5 (2%)	1 (0%)	29	52
4	L	214/217 (99%)	203 (95%)	9 (4%)	2 (1%)	17	35
All	All	2566/2762 (93%)	2441 (95%)	117 (5%)	8 (0%)	41	64



5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
4	K	72	ARG
2	D	171	GLY
2	B	409	LYS
1	C	265	LYS

### 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	374/407 (92%)	369 (99%)	5 (1%)	69	86
1	C	378/407 (93%)	378 (100%)	0	100	100
2	B	404/428 (94%)	398 (98%)	6 (2%)	65	83
2	D	392/428 (92%)	389 (99%)	3 (1%)	81	92
3	H	189/192 (98%)	187 (99%)	2 (1%)	73	88
3	J	189/192 (98%)	184 (97%)	5 (3%)	46	72
4	K	190/191 (100%)	188 (99%)	2 (1%)	73	88
4	L	190/191 (100%)	186 (98%)	4 (2%)	53	77
All	All	2306/2436 (95%)	2279 (99%)	27 (1%)	71	87

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	206	LYS
3	H	17	SER
3	J	198	THR
2	D	274	PHE
1	A	364	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	398	HIS
2	D	22	ASN
4	L	161	ASN
1	C	220	GLN
4	L	149	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](#)

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	905	1	14,14,15	0.67	0	17,19,21	1.54	1 (5%)
5	NAG	A	902	1	14,14,15	0.55	0	17,19,21	1.05	1 (5%)
5	NAG	B	907	2	14,14,15	0.44	0	17,19,21	1.62	1 (5%)
5	NAG	A	907	1	14,14,15	0.57	0	17,19,21	1.08	1 (5%)
5	NAG	B	902	2	14,14,15	0.61	0	17,19,21	0.90	0
5	NAG	A	906	1	14,14,15	0.70	0	17,19,21	0.98	0
5	NAG	C	902	1	14,14,15	0.54	0	17,19,21	0.86	1 (5%)
5	NAG	B	901	2	14,14,15	1.24	2 (14%)	17,19,21	1.75	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	908	1	14,14,15	0.53	0	17,19,21	1.19	2 (11%)
5	NAG	B	904	2	14,14,15	0.47	0	17,19,21	1.62	3 (17%)
5	NAG	A	904	1	14,14,15	0.53	0	17,19,21	0.92	1 (5%)
5	NAG	B	905	2	14,14,15	0.56	0	17,19,21	0.90	0
5	NAG	B	906	2	14,14,15	0.45	0	17,19,21	1.92	2 (11%)
5	NAG	D	902	2	14,14,15	0.47	0	17,19,21	2.19	3 (17%)
5	NAG	C	906	1	14,14,15	0.86	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	A	901	1	14,14,15	0.74	0	17,19,21	1.70	5 (29%)
5	NAG	D	903	2	14,14,15	0.51	0	17,19,21	1.33	2 (11%)
5	NAG	B	903	2	14,14,15	0.48	0	17,19,21	1.05	1 (5%)
5	NAG	C	903	1	14,14,15	0.54	0	17,19,21	1.04	1 (5%)
5	NAG	A	903	1	14,14,15	0.55	0	17,19,21	1.19	1 (5%)
5	NAG	C	907	1	14,14,15	0.37	0	17,19,21	2.08	6 (35%)
5	NAG	D	901	2	14,14,15	0.48	0	17,19,21	0.92	0
5	NAG	C	901	1	14,14,15	0.74	0	17,19,21	1.47	3 (17%)
5	NAG	C	905	1	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
5	NAG	D	904	2	14,14,15	0.63	0	17,19,21	2.05	6 (35%)
5	NAG	C	904	1	14,14,15	0.73	0	17,19,21	1.19	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	905	1	-	4/6/23/26	0/1/1/1
5	NAG	A	902	1	-	2/6/23/26	0/1/1/1
5	NAG	B	907	2	-	4/6/23/26	0/1/1/1
5	NAG	A	907	1	-	2/6/23/26	0/1/1/1
5	NAG	B	902	2	-	2/6/23/26	0/1/1/1
5	NAG	A	906	1	-	2/6/23/26	0/1/1/1
5	NAG	C	902	1	-	2/6/23/26	0/1/1/1
5	NAG	B	901	2	-	4/6/23/26	0/1/1/1
5	NAG	C	908	1	-	2/6/23/26	0/1/1/1
5	NAG	B	904	2	-	4/6/23/26	0/1/1/1
5	NAG	A	904	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	905	2	-	3/6/23/26	0/1/1/1
5	NAG	B	906	2	-	3/6/23/26	0/1/1/1
5	NAG	D	902	2	-	4/6/23/26	0/1/1/1
5	NAG	C	906	1	-	4/6/23/26	0/1/1/1
5	NAG	A	901	1	-	2/6/23/26	0/1/1/1
5	NAG	D	903	2	-	2/6/23/26	0/1/1/1
5	NAG	B	903	2	-	4/6/23/26	0/1/1/1
5	NAG	C	903	1	-	4/6/23/26	0/1/1/1
5	NAG	A	903	1	-	4/6/23/26	0/1/1/1
5	NAG	C	907	1	-	3/6/23/26	0/1/1/1
5	NAG	D	901	2	-	2/6/23/26	0/1/1/1
5	NAG	C	901	1	-	2/6/23/26	0/1/1/1
5	NAG	C	905	1	-	2/6/23/26	0/1/1/1
5	NAG	D	904	2	-	2/6/23/26	0/1/1/1
5	NAG	C	904	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	NAG	O5-C1	-2.98	1.39	1.43
5	B	901	NAG	O5-C5	-2.69	1.38	1.43
5	C	906	NAG	O5-C1	-2.06	1.40	1.43

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	902	NAG	C1-O5-C5	7.00	121.68	112.19
5	B	906	NAG	C1-O5-C5	6.20	120.59	112.19
5	B	907	NAG	C1-O5-C5	6.13	120.49	112.19
5	A	905	NAG	C1-O5-C5	5.87	120.14	112.19
5	C	907	NAG	C1-O5-C5	5.78	120.03	112.19

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	903	NAG	O5-C5-C6-O6
5	B	903	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	905	NAG	O5-C5-C6-O6
5	B	904	NAG	C4-C5-C6-O6
5	C	903	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	902	NAG	1	0
5	B	902	NAG	1	0
5	B	906	NAG	1	1
5	A	901	NAG	1	0
5	D	903	NAG	1	0
5	C	907	NAG	1	0

## 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, 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	A	421/461 (91%)	-0.10	3 (0%) 87 86	23, 38, 60, 72	0
1	C	426/461 (92%)	-0.12	6 (1%) 75 71	22, 35, 59, 77	0
2	B	452/478 (94%)	0.12	12 (2%) 54 48	29, 53, 79, 94	0
2	D	441/478 (92%)	0.13	21 (4%) 30 24	23, 48, 91, 109	0
3	H	219/225 (97%)	0.04	2 (0%) 84 82	21, 44, 69, 80	0
3	J	220/225 (97%)	-0.04	6 (2%) 54 48	23, 41, 66, 80	0
4	K	216/217 (99%)	-0.18	1 (0%) 91 89	22, 34, 52, 66	0
4	L	216/217 (99%)	-0.19	1 (0%) 91 89	18, 39, 65, 78	0
All	All	2611/2762 (94%)	-0.02	52 (1%) 65 60	18, 41, 73, 109	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	259	ILE	6.7
3	J	200	PRO	4.4
3	J	199	TRP	4.4
1	C	25	THR	4.3
2	B	365	SER	4.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	NA	C	962	1/1	0.60	0.25	54,54,54,54	0
5	NAG	B	904	14/15	0.63	0.35	86,100,102,106	0
5	NAG	C	908	14/15	0.63	0.36	60,76,86,88	0
5	NAG	A	903	14/15	0.63	0.31	92,100,112,115	0
5	NAG	D	904	14/15	0.66	0.48	85,101,115,117	0
5	NAG	B	901	14/15	0.69	0.42	103,119,124,126	0
5	NAG	C	902	14/15	0.71	0.34	88,100,110,118	0
5	NAG	B	906	14/15	0.74	0.27	89,99,104,104	0
5	NAG	B	903	14/15	0.74	0.29	88,101,113,113	0
5	NAG	B	907	14/15	0.75	0.27	85,97,105,107	0
5	NAG	C	903	14/15	0.75	0.27	66,78,81,82	0
5	NAG	A	902	14/15	0.77	0.45	103,115,126,127	0
5	NAG	A	905	14/15	0.80	0.22	71,86,95,97	0
5	NAG	B	905	14/15	0.80	0.49	80,93,109,116	0
5	NAG	A	907	14/15	0.81	0.26	72,85,97,99	0
5	NAG	C	905	14/15	0.82	0.24	52,63,72,75	0
5	NAG	D	903	14/15	0.83	0.18	43,62,71,73	0
6	ARG	B	951[B]	12/12	0.83	0.33	35,70,78,81	8
6	ARG	B	951[A]	12/12	0.83	0.33	35,71,78,81	8
6	ARG	D	951[A]	12/12	0.85	0.38	29,59,81,88	8
7	NA	A	962	1/1	0.85	0.16	60,60,60,60	0
6	ARG	D	951[B]	12/12	0.85	0.38	29,64,82,88	8
5	NAG	C	907	14/15	0.86	0.24	58,67,79,85	0
5	NAG	A	904	14/15	0.86	0.23	50,62,75,78	0
5	NAG	B	902	14/15	0.87	0.17	38,52,61,64	0
5	NAG	D	901	14/15	0.89	0.17	39,52,68,70	0
5	NAG	A	906	14/15	0.90	0.19	37,51,61,66	0
7	NA	C	961	1/1	0.90	0.24	37,37,37,37	0
7	NA	A	961	1/1	0.91	0.10	34,34,34,34	0
7	NA	D	961	1/1	0.91	0.10	37,37,37,37	0
5	NAG	D	902	14/15	0.93	0.17	33,48,53,55	0
5	NAG	C	904	14/15	0.93	0.25	45,53,63,66	0
5	NAG	C	906	14/15	0.94	0.11	34,41,52,61	0
5	NAG	C	901	14/15	0.95	0.13	19,28,36,39	0
5	NAG	A	901	14/15	0.96	0.14	17,33,43,50	0
6	ARG	C	951	12/12	0.96	0.19	22,28,33,34	0
8	CL	D	971	1/1	0.97	0.34	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CA	K	301	1/1	0.97	0.13	50,50,50,50	0
6	ARG	A	951	12/12	0.98	0.18	20,30,35,37	0
8	CL	B	971	1/1	0.99	0.22	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.