



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 12:58 PM BST

PDB ID : 5X2M  
Title : Crystal structure of the medaka fish taste receptor T1r2a-T1r3 ligand binding domains in complex with L-glutamine  
Authors : Nuemket, N.; Yasui, N.; Atsumi, N.; Yamashita, A.  
Deposited on : 2017-02-02  
Resolution : 2.21 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.

---

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

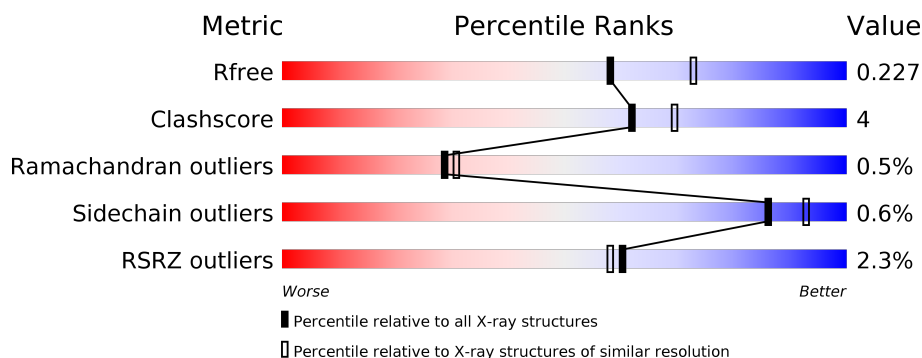
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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.



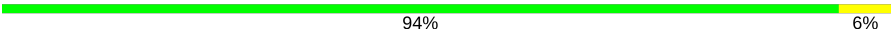

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>87%</span> <span>7%</span> <span>7%</span> </div> </div>
1	C	461	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>84%</span> <span>8%</span> <span>7%</span> </div> </div>
2	B	478	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>84%</span> <span>11%</span> <span>5%</span> </div> </div>
2	D	478	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>71%</span> <span>17%</span> <span>• 12%</span> </div> </div>
3	H	225	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>89%</span> <span>8%</span> <span>•</span> </div> </div>
3	J	225	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>10%</span> <span>• •</span> </div> </div>

Continued on next page...

*Continued from previous page...*

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	D	905	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21519 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	429	Total	C	N	O	S	0	2	0
			3413	2206	565	624	18			
1	C	427	Total	C	N	O	S	0	1	0
			3388	2186	562	622	18			

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	2	0
			3557	2287	570	685	15			
2	D	422	Total	C	N	O	S	0	1	0
			3304	2123	531	637	13			

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	217	Total	C	N	O	S	0	0	0
			1647	1048	271	320	8			

- Molecule 4 is a protein called Fab16A Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	217	Total	C	N	O	S	0	0	0
			1679	1040	288	345	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>).



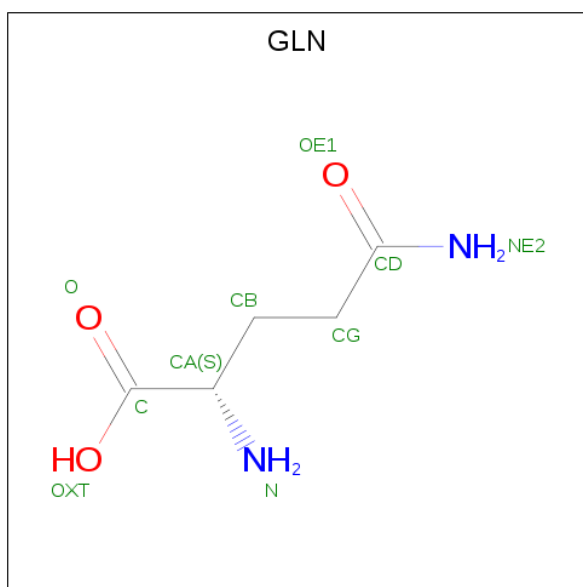
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1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

Continued on next page...

*Continued from previous page...*

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		
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 GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			10	5	2	3		
6	B	1	Total	C	N	O	0	0
			10	5	2	3		
6	C	1	Total	C	N	O	0	0
			10	5	2	3		
6	D	1	Total	C	N	O	0	0
			10	5	2	3		

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

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

- 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		



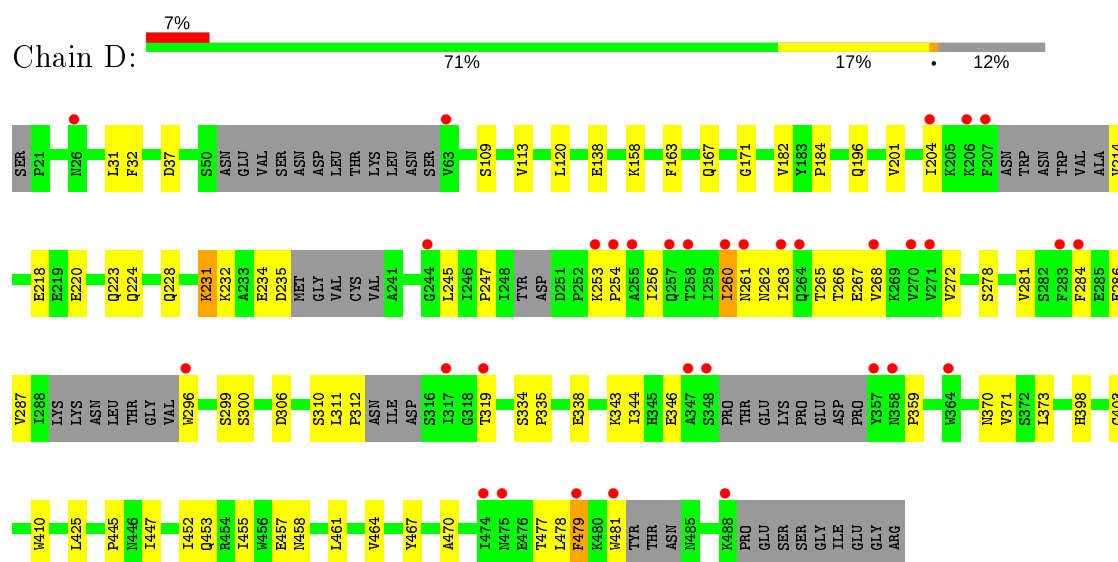
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

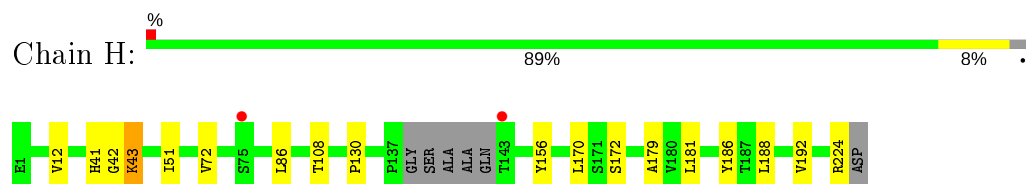
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	191	Total 191	O 191	0	0
10	B	100	Total 100	O 100	0	0
10	C	149	Total 149	O 149	0	0
10	D	46	Total 46	O 46	0	0
10	H	81	Total 81	O 81	0	0
10	L	73	Total 73	O 73	0	0
10	J	47	Total 47	O 47	0	0
10	K	88	Total 88	O 88	0	0

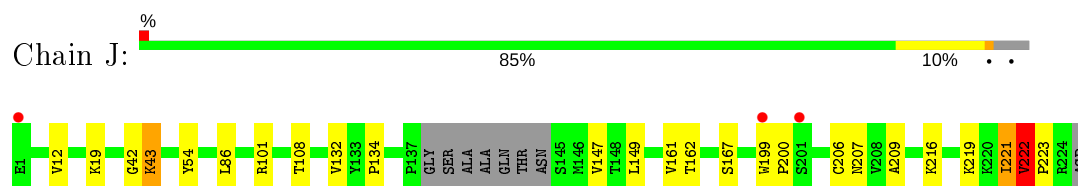




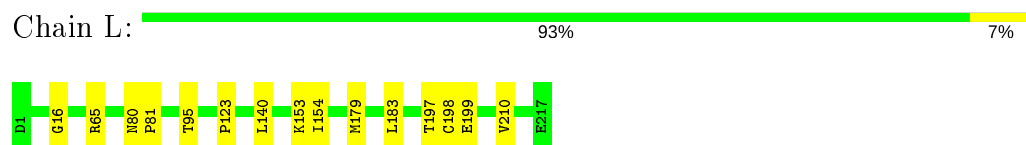
- Molecule 3: Fab16A Heavy chain



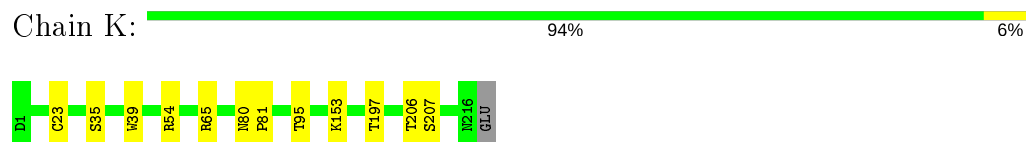
- Molecule 3: Fab16A Heavy chain



- 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, $\alpha$ , $\beta$ , $\gamma$	99.66 Å 116.36 Å 129.48 Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	49.89 – 2.21 49.89 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.89-2.21) 96.2 (49.89-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.20 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.173 , 0.227 0.175 , 0.227	Depositor DCC
$R_{free}$ test set	7155 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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](#)

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	0/3507	0.55	0/4761
1	C	0.43	0/3478	0.53	0/4722
2	B	0.39	0/3645	0.52	0/4957
2	D	0.38	0/3375	0.53	0/4575
3	H	0.41	0/1706	0.55	0/2331
3	J	0.40	0/1691	0.60	2/2310 (0.1%)
4	K	0.41	0/1707	0.55	0/2320
4	L	0.44	0/1716	0.55	0/2332
All	All	0.42	0/20825	0.54	2/28308 (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
3	J	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	222	VAL	C-N-CD	-6.96	105.28	120.60
3	J	222	VAL	C-N-CA	5.61	145.55	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	221	ILE	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	3413	0	3343	20	0
1	C	3388	0	3311	25	0
2	B	3557	0	3511	37	0
2	D	3304	0	3255	58	1
3	H	1662	0	1642	11	0
3	J	1647	0	1629	20	0
4	K	1670	0	1596	6	1
4	L	1679	0	1602	9	0
5	A	98	0	91	2	0
5	B	98	0	91	2	0
5	C	98	0	91	3	0
5	D	84	0	78	3	0
6	A	10	0	7	0	0
6	B	10	0	7	4	0
6	C	10	0	7	0	0
6	D	10	0	7	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	L	1	0	0	0	0
10	A	191	0	0	4	0
10	B	100	0	0	7	0
10	C	149	0	0	2	0
10	D	46	0	0	6	0
10	H	81	0	0	1	0
10	J	47	0	0	3	0
10	K	88	0	0	0	0
10	L	73	0	0	0	0
All	All	21519	0	20268	181	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 4.

The worst 5 of 181 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)
2:D:479:PHE:HB3	2:D:481:TRP:HE1	1.23	1.02
3:J:167:SER:H	3:J:207:ASN:HD21	1.19	0.87
2:B:92:LEU:O	2:B:398:HIS:ND1	2.07	0.87
2:B:334:SER:O	10:B:1001:HOH:O	1.97	0.82
2:D:455:ILE:HD13	5:D:903:NAG:H83	1.63	0.81

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)
2:D:310:SER:OG	4:K:206:THR:O[2_846]	2.18	0.02

## 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	425/461 (92%)	409 (96%)	15 (4%)	1 (0%)	47	55
1	C	422/461 (92%)	403 (96%)	17 (4%)	2 (0%)	29	31
2	B	448/478 (94%)	437 (98%)	9 (2%)	2 (0%)	34	37
2	D	405/478 (85%)	382 (94%)	17 (4%)	6 (2%)	10	8
3	H	215/225 (96%)	209 (97%)	5 (2%)	1 (0%)	29	31
3	J	213/225 (95%)	205 (96%)	6 (3%)	2 (1%)	17	16
4	K	214/217 (99%)	207 (97%)	7 (3%)	0	100	100
4	L	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
All	All	2557/2762 (93%)	2459 (96%)	84 (3%)	14 (0%)	29	31

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	231	LYS
3	J	43	LYS
2	B	250	ASP
1	C	117	ASN
2	D	267	GLU

### 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	384/407 (94%)	384 (100%)	0	100	100
1	C	381/407 (94%)	378 (99%)	3 (1%)	81	90
2	B	406/428 (95%)	402 (99%)	4 (1%)	76	86
2	D	376/428 (88%)	374 (100%)	2 (0%)	88	94
3	H	189/192 (98%)	188 (100%)	1 (0%)	88	94
3	J	187/192 (97%)	185 (99%)	2 (1%)	73	85
4	K	190/191 (100%)	189 (100%)	1 (0%)	88	94
4	L	191/191 (100%)	190 (100%)	1 (0%)	88	94
All	All	2304/2436 (95%)	2290 (99%)	14 (1%)	86	93

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	352	ASN
2	D	261	ASN
3	J	161	VAL
1	C	331	SER
4	L	198	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:



Mol	Chain	Res	Type
2	D	148	GLN
2	D	167	GLN
3	J	41	HIS
2	D	26	ASN
4	L	214	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 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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	C	905	1	14,14,15	0.57	0	17,19,21	1.56	2 (11%)
5	NAG	A	905	1	14,14,15	0.50	0	17,19,21	1.28	1 (5%)
5	NAG	A	904	1	14,14,15	0.47	0	17,19,21	1.53	1 (5%)
5	NAG	B	902	2	14,14,15	0.50	0	17,19,21	1.37	3 (17%)
5	NAG	A	902	1	14,14,15	0.55	0	17,19,21	1.07	1 (5%)
5	NAG	A	906	1	14,14,15	0.51	0	17,19,21	1.05	1 (5%)
5	NAG	D	903	2	14,14,15	0.39	0	17,19,21	1.73	3 (17%)
5	NAG	A	903	1	14,14,15	0.56	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	D	906	2	14,14,15	0.46	0	17,19,21	1.17	2 (11%)
5	NAG	D	902	2	14,14,15	0.53	0	17,19,21	1.83	3 (17%)
5	NAG	D	905	2	14,14,15	0.73	0	17,19,21	1.61	3 (17%)
5	NAG	A	901	1	14,14,15	0.57	0	17,19,21	1.47	2 (11%)
5	NAG	D	904	2	14,14,15	0.50	0	17,19,21	0.66	0
5	NAG	B	904	2	14,14,15	0.43	0	17,19,21	2.34	2 (11%)
5	NAG	B	903	2	14,14,15	0.48	0	17,19,21	1.31	1 (5%)
5	NAG	C	904	1	14,14,15	0.52	0	17,19,21	1.27	2 (11%)
5	NAG	D	901	2	14,14,15	0.47	0	17,19,21	1.14	1 (5%)
5	NAG	B	901	2	14,14,15	0.63	0	17,19,21	0.92	1 (5%)
5	NAG	A	907	1	14,14,15	0.54	0	17,19,21	0.98	2 (11%)
5	NAG	B	906	2	14,14,15	0.49	0	17,19,21	0.74	1 (5%)
5	NAG	C	901	1	14,14,15	0.54	0	17,19,21	1.26	2 (11%)
5	NAG	B	907	2	14,14,15	0.79	1 (7%)	17,19,21	1.63	3 (17%)
5	NAG	C	902	1	14,14,15	0.56	0	17,19,21	0.79	0
5	NAG	C	903	1	14,14,15	0.48	0	17,19,21	1.14	1 (5%)
5	NAG	C	907	1	14,14,15	0.54	0	17,19,21	1.10	2 (11%)
5	NAG	B	905	2	14,14,15	0.47	0	17,19,21	1.51	2 (11%)
5	NAG	C	906	1	14,14,15	0.53	0	17,19,21	1.11	3 (17%)

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	C	905	1	-	3/6/23/26	0/1/1/1
5	NAG	A	905	1	-	4/6/23/26	0/1/1/1
5	NAG	A	904	1	-	2/6/23/26	0/1/1/1
5	NAG	B	902	2	-	4/6/23/26	0/1/1/1
5	NAG	A	902	1	-	2/6/23/26	0/1/1/1
5	NAG	A	906	1	-	4/6/23/26	0/1/1/1
5	NAG	D	903	2	-	2/6/23/26	0/1/1/1
5	NAG	A	903	1	-	4/6/23/26	0/1/1/1
5	NAG	D	906	2	-	2/6/23/26	0/1/1/1
5	NAG	D	902	2	-	4/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	907	NAG	O5-C1	-2.06	1.40	1.43

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	904	NAG	C1-O5-C5	8.08	123.14	112.19
5	D	903	NAG	C1-O5-C5	5.40	119.50	112.19
5	D	902	NAG	C1-O5-C5	5.37	119.47	112.19
5	A	904	NAG	C1-O5-C5	5.22	119.26	112.19
5	C	905	NAG	C1-O5-C5	5.13	119.14	112.19

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	904	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	903	NAG	O5-C5-C6-O6
5	A	905	NAG	O5-C5-C6-O6
5	B	901	NAG	O5-C5-C6-O6
5	D	902	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	903	NAG	1	0
5	D	902	NAG	2	0
5	A	901	NAG	2	0
5	B	904	NAG	1	0
5	B	903	NAG	1	0
5	C	904	NAG	1	0
5	C	901	NAG	1	0
5	C	903	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	429/461 (93%)	-0.35	4 (0%) 84 83	26, 39, 74, 126	0
1	C	427/461 (92%)	-0.32	8 (1%) 66 65	29, 42, 77, 130	0
2	B	452/478 (94%)	-0.25	10 (2%) 62 59	28, 50, 83, 123	0
2	D	422/478 (88%)	0.21	33 (7%) 13 11	33, 61, 116, 149	0
3	H	219/225 (97%)	-0.56	2 (0%) 84 83	28, 47, 74, 112	0
3	J	217/225 (96%)	-0.46	3 (1%) 75 73	31, 51, 84, 121	0
4	K	216/217 (99%)	-0.71	0 100 100	31, 41, 64, 92	0
4	L	217/217 (100%)	-0.62	0 100 100	27, 45, 69, 92	0
All	All	2599/2762 (94%)	-0.32	60 (2%) 60 58	26, 47, 93, 149	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	260	ILE	7.8
2	D	263	ILE	5.3
2	B	364	TRP	4.7
2	B	357	TYR	4.2
2	D	296	TRP	4.0

### 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
5	NAG	D	905	14/15	0.49	0.53	124,144,156,156	0
5	NAG	D	906	14/15	0.68	0.38	112,120,126,129	0
5	NAG	B	901	14/15	0.71	0.32	94,110,121,123	0
5	NAG	B	906	14/15	0.73	0.35	94,106,113,116	0
5	NAG	B	905	14/15	0.74	0.35	96,115,123,127	0
5	NAG	C	902	14/15	0.75	0.29	94,108,123,128	0
5	NAG	D	904	14/15	0.77	0.28	98,111,118,118	0
5	NAG	B	904	14/15	0.77	0.21	101,111,121,124	0
5	NAG	C	903	14/15	0.79	0.19	70,79,93,94	0
5	NAG	B	907	14/15	0.82	0.29	89,99,105,107	0
5	NAG	A	905	14/15	0.82	0.21	77,89,91,96	0
9	CA	L	971	1/1	0.83	0.24	97,97,97,97	0
5	NAG	D	903	14/15	0.85	0.25	81,107,114,116	0
5	NAG	A	902	14/15	0.87	0.39	88,101,105,107	0
5	NAG	C	905	14/15	0.88	0.15	72,86,93,96	0
7	NA	D	961	1/1	0.90	0.06	60,60,60,60	0
5	NAG	D	902	14/15	0.91	0.16	45,63,75,82	0
5	NAG	A	907	14/15	0.91	0.23	88,111,114,118	0
5	NAG	A	903	14/15	0.91	0.15	75,89,103,104	0
5	NAG	B	903	14/15	0.91	0.22	77,94,105,106	0
5	NAG	C	907	14/15	0.92	0.17	46,64,79,88	0
5	NAG	B	902	14/15	0.93	0.11	39,56,70,75	0
5	NAG	A	904	14/15	0.93	0.13	55,66,72,80	0
5	NAG	A	906	14/15	0.93	0.12	49,57,66,67	0
5	NAG	C	906	14/15	0.93	0.08	47,58,67,68	0
7	NA	A	961	1/1	0.94	0.06	41,41,41,41	0
5	NAG	C	904	14/15	0.94	0.18	53,68,80,81	0
6	GLN	D	951	10/10	0.95	0.18	43,49,78,84	0
6	GLN	B	951	10/10	0.96	0.17	29,38,68,78	0
5	NAG	D	901	14/15	0.96	0.14	49,62,79,83	0
8	CL	B	971	1/1	0.97	0.41	79,79,79,79	0
5	NAG	C	901	14/15	0.97	0.09	28,41,47,59	0
5	NAG	A	901	14/15	0.98	0.09	28,37,44,50	0
7	NA	C	961	1/1	0.98	0.10	39,39,39,39	0
6	GLN	A	951	10/10	0.98	0.17	26,29,39,39	0
6	GLN	C	951	10/10	0.98	0.16	24,33,39,43	0
8	CL	D	971	1/1	0.99	0.12	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.