



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:36 PM UTC

PDB ID : 5X2O / pdb_00005x2o
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

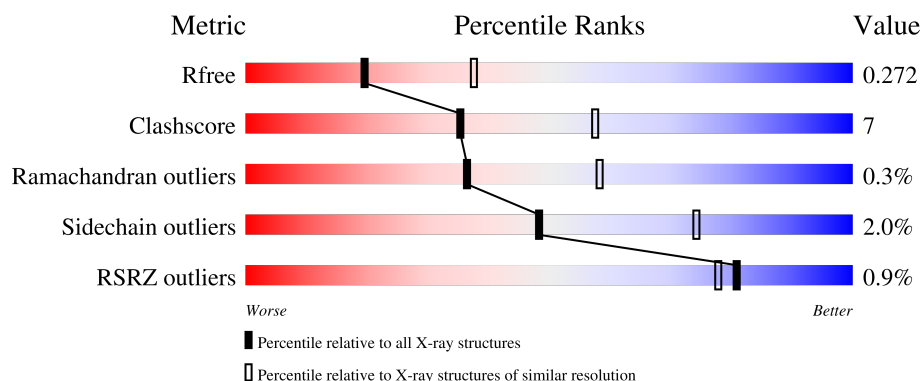
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	461	 77% 13% • 9%
1	C	461	 77% 16% 8%
2	B	478	 % 73% 21% • 5%
2	D	478	 3% 69% 22% • 8%
3	H	225	 % 81% 16% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	225	2% 78% 18%
4	K	217	85% 15%
4	L	217	88% 12%

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

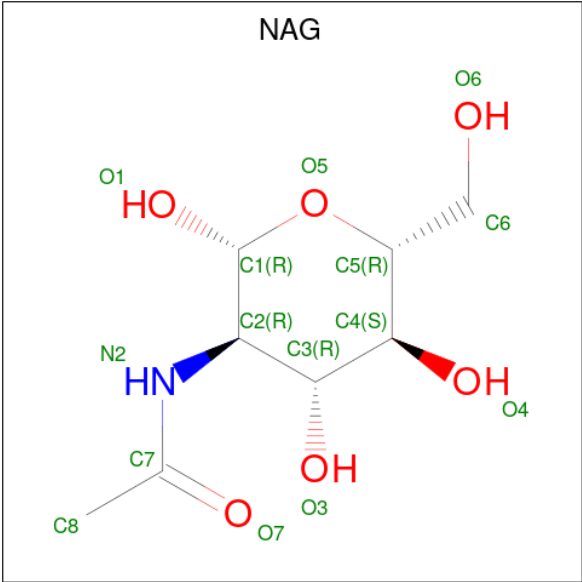
- Molecule 3 is a protein called Fab16A Heavy chain.

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



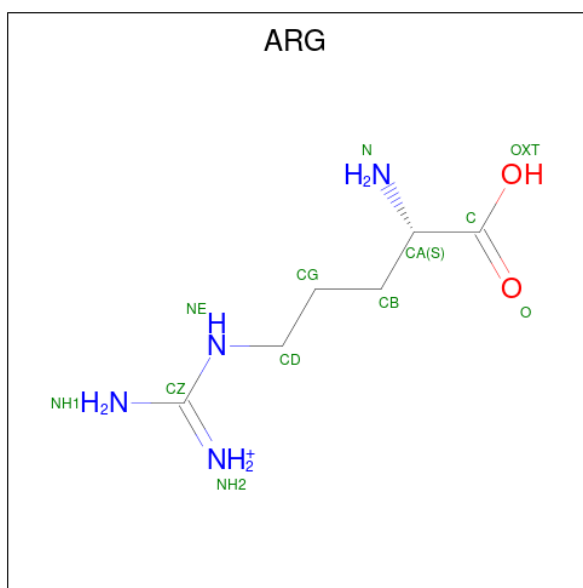
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1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

- Molecule 6 is ARGinine (CCD ID: 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 (CCD ID: NA) (formula: Na).

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

- Molecule 8 is CHLORIDE ION (CCD ID: 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 (CCD ID: 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		

Continued on next page...

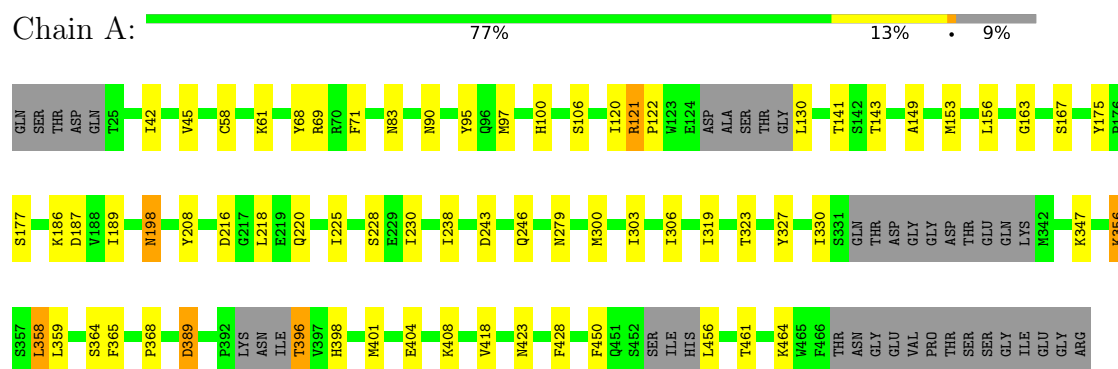
Continued from previous page...

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.

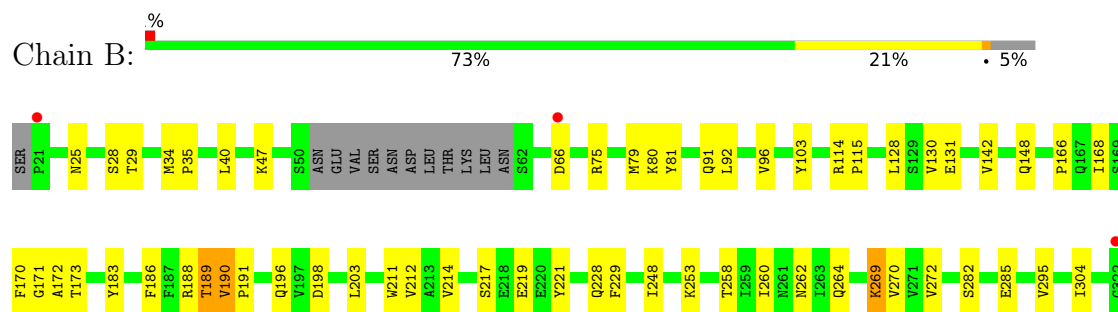
- Molecule 1: Taste receptor, type 1, member 2a

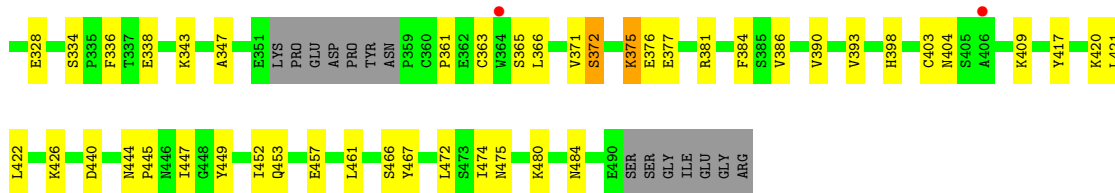


- Molecule 1: Taste receptor, type 1, member 2a

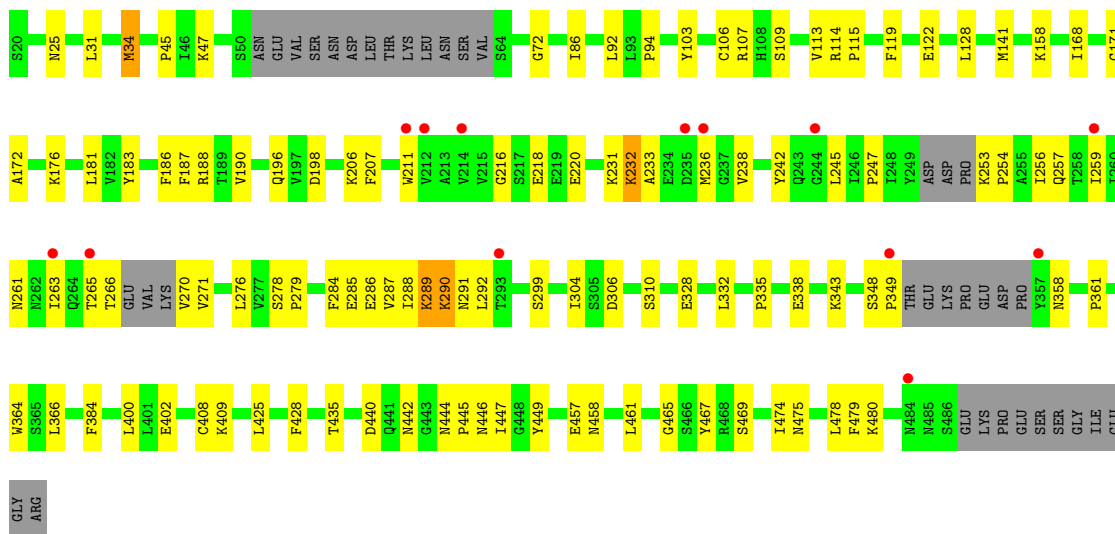


- Molecule 2: Taste receptor, type 1, member 3

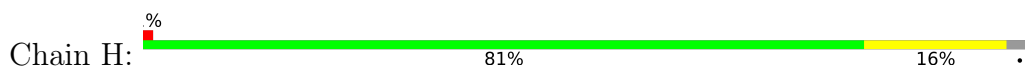




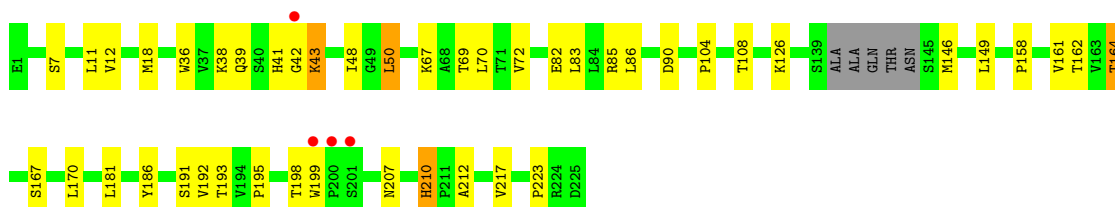
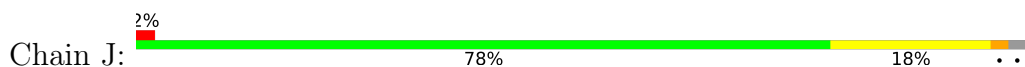
• Molecule 2: Taste receptor, type 1, member 3



• Molecule 3: Fab16A Heavy chain



• Molecule 3: Fab16A Heavy chain



• Molecule 4: Fab16A Light chain

Chain L:

88%

12%

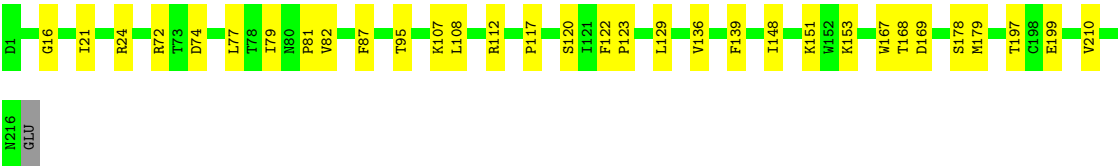


● Molecule 4: Fab16A Light chain

Chain K:

85%

15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.91Å 113.68Å 128.64Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	49.41 – 2.60 49.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (49.41-2.60) 95.9 (49.41-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

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

5.1 Standard geometry

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

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	0.56	0/3423	0.88	4/4646 (0.1%)
1	C	0.60	0/3458	0.89	3/4695 (0.1%)
2	B	0.53	0/3621	0.88	5/4923 (0.1%)
2	D	0.52	0/3529	0.90	8/4797 (0.2%)
3	H	0.54	0/1706	0.84	2/2331 (0.1%)
3	J	0.56	0/1709	0.91	3/2334 (0.1%)
4	K	0.55	0/1707	0.85	0/2320
4	L	0.54	0/1707	0.86	2/2320 (0.1%)
All	All	0.55	0/20860	0.88	27/28366 (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
2	D	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	CA-C-N	9.40	129.15	119.56
1	A	121	ARG	C-N-CA	9.40	129.15	119.56
2	D	358	ASN	CA-C-N	9.36	129.57	119.28
2	D	358	ASN	C-N-CA	9.36	129.57	119.28
2	D	183	TYR	CA-C-N	7.35	126.98	119.56

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	40	0
1	C	3370	0	3290	50	0
2	B	3540	0	3495	64	0
2	D	3451	0	3409	77	0
3	H	1662	0	1642	23	0
3	J	1665	0	1641	27	1
4	K	1670	0	1596	19	0
4	L	1670	0	1596	14	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	24	0	0	1	0
10	L	34	0	0	0	0
All	All	21165	0	20337	306	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 306 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	1.44	0.81
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%)	24 46
1	C	419/461 (91%)	399 (95%)	19 (4%)	1 (0%)	43 66
2	B	446/478 (93%)	420 (94%)	25 (6%)	1 (0%)	43 66
2	D	431/478 (90%)	404 (94%)	26 (6%)	1 (0%)	43 66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	46
4	L	214/217 (99%)	203 (95%)	9 (4%)	2 (1%)	14	30
All	All	2566/2762 (93%)	2441 (95%)	117 (5%)	8 (0%)	36	58

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%)	363 (97%)	11 (3%)	37	65
1	C	378/407 (93%)	378 (100%)	0	100	100
2	B	404/428 (94%)	393 (97%)	11 (3%)	39	67
2	D	392/428 (92%)	386 (98%)	6 (2%)	57	80
3	H	189/192 (98%)	187 (99%)	2 (1%)	65	84
3	J	189/192 (98%)	182 (96%)	7 (4%)	30	57
4	K	190/191 (100%)	186 (98%)	4 (2%)	47	73
4	L	190/191 (100%)	185 (97%)	5 (3%)	40	68
All	All	2306/2436 (95%)	2260 (98%)	46 (2%)	48	74

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	7	SER
3	J	7	SER
3	H	17	SER
4	L	199	GLU
3	J	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	22	ASN
2	D	345	HIS
2	D	262	ASN
3	H	166	ASN
1	C	220	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 oligosaccharides 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	B	905	2	14,14,15	0.55	0	17,19,21	0.86	0
5	NAG	C	905	1	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
5	NAG	A	907	1	14,14,15	0.58	0	17,19,21	1.05	1 (5%)
5	NAG	D	903	2	14,14,15	0.50	0	17,19,21	1.22	2 (11%)
5	NAG	A	906	1	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
5	NAG	A	904	1	14,14,15	0.53	0	17,19,21	0.93	1 (5%)
5	NAG	C	904	1	14,14,15	0.71	0	17,19,21	1.22	1 (5%)
5	NAG	D	902	2	14,14,15	0.45	0	17,19,21	2.20	3 (17%)
6	ARG	B	951[B]	-	10,11,11	0.77	1 (10%)	9,13,13	1.03	1 (11%)
5	NAG	C	908	1	14,14,15	0.52	0	17,19,21	1.22	2 (11%)
5	NAG	A	903	1	14,14,15	0.57	0	17,19,21	1.19	1 (5%)
5	NAG	B	903	2	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
5	NAG	A	902	1	14,14,15	0.54	0	17,19,21	1.04	1 (5%)
5	NAG	B	907	2	14,14,15	0.43	0	17,19,21	1.64	1 (5%)
5	NAG	C	903	1	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
5	NAG	B	906	2	14,14,15	0.44	0	17,19,21	1.93	2 (11%)
5	NAG	C	906	1	14,14,15	0.84	0	17,19,21	0.98	1 (5%)
5	NAG	B	904	2	14,14,15	0.45	0	17,19,21	1.57	4 (23%)
5	NAG	B	902	2	14,14,15	0.61	0	17,19,21	0.86	0
5	NAG	D	904	2	14,14,15	0.61	0	17,19,21	2.03	7 (41%)
5	NAG	A	901	1	14,14,15	0.72	0	17,19,21	1.65	4 (23%)
6	ARG	D	951[A]	-	10,11,11	0.84	1 (10%)	9,13,13	1.43	1 (11%)
5	NAG	C	907	1	14,14,15	0.35	0	17,19,21	2.08	5 (29%)
5	NAG	C	902	1	14,14,15	0.52	0	17,19,21	0.82	1 (5%)
6	ARG	C	951	-	10,11,11	0.81	1 (10%)	9,13,13	1.20	1 (11%)
6	ARG	D	951[B]	-	10,11,11	0.77	1 (10%)	9,13,13	1.39	1 (11%)
5	NAG	B	901	2	14,14,15	1.23	2 (14%)	17,19,21	1.70	4 (23%)
5	NAG	A	905	1	14,14,15	0.66	0	17,19,21	1.55	1 (5%)
6	ARG	B	951[A]	-	10,11,11	0.78	1 (10%)	9,13,13	1.12	1 (11%)
5	NAG	C	901	1	14,14,15	0.72	0	17,19,21	1.32	3 (17%)
6	ARG	A	951	-	10,11,11	0.72	0	9,13,13	0.80	0
5	NAG	D	901	2	14,14,15	0.47	0	17,19,21	0.88	0

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	B	905	2	-	3/6/23/26	0/1/1/1
5	NAG	C	905	1	-	2/6/23/26	0/1/1/1
5	NAG	A	907	1	-	2/6/23/26	0/1/1/1
5	NAG	D	903	2	-	2/6/23/26	0/1/1/1
5	NAG	A	906	1	-	2/6/23/26	0/1/1/1
5	NAG	A	904	1	-	2/6/23/26	0/1/1/1
5	NAG	C	904	1	-	2/6/23/26	0/1/1/1
5	NAG	D	902	2	-	4/6/23/26	0/1/1/1
6	ARG	B	951[B]	-	-	2/11/11/11	-
5	NAG	C	908	1	-	2/6/23/26	0/1/1/1
5	NAG	A	903	1	-	4/6/23/26	0/1/1/1
5	NAG	B	903	2	-	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	C	903	1	-	4/6/23/26	0/1/1/1
5	NAG	B	906	2	-	3/6/23/26	0/1/1/1
5	NAG	C	906	1	-	4/6/23/26	0/1/1/1
5	NAG	B	904	2	-	4/6/23/26	0/1/1/1
5	NAG	B	902	2	-	2/6/23/26	0/1/1/1
5	NAG	D	904	2	-	2/6/23/26	0/1/1/1
5	NAG	A	901	1	-	2/6/23/26	0/1/1/1
6	ARG	D	951[A]	-	-	2/11/11/11	-
5	NAG	C	907	1	-	3/6/23/26	0/1/1/1
5	NAG	C	902	1	-	2/6/23/26	0/1/1/1
6	ARG	C	951	-	-	1/11/11/11	-
6	ARG	D	951[B]	-	-	2/11/11/11	-
5	NAG	B	901	2	-	4/6/23/26	0/1/1/1
5	NAG	A	905	1	-	4/6/23/26	0/1/1/1
6	ARG	B	951[A]	-	-	4/11/11/11	-
5	NAG	C	901	1	-	2/6/23/26	0/1/1/1
6	ARG	A	951	-	-	0/11/11/11	-
5	NAG	D	901	2	-	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	NAG	O5-C1	-2.82	1.39	1.43
5	B	901	NAG	O5-C5	-2.79	1.38	1.43
6	C	951	ARG	OXT-C	-2.43	1.22	1.30
6	B	951[A]	ARG	OXT-C	-2.25	1.23	1.30
6	B	951[B]	ARG	OXT-C	-2.25	1.23	1.30

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	902	NAG	C1-O5-C5	7.08	121.68	112.19
5	B	906	NAG	C1-O5-C5	6.27	120.59	112.19
5	B	907	NAG	C1-O5-C5	6.20	120.49	112.19
5	A	905	NAG	C1-O5-C5	5.94	120.14	112.19
5	C	907	NAG	C1-O5-C5	5.85	120.03	112.19

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	951[A]	ARG	N-CA-CB-CG
6	B	951[B]	ARG	N-CA-CB-CG
6	D	951[B]	ARG	CA-CB-CG-CD
5	C	903	NAG	O5-C5-C6-O6
6	B	951[A]	ARG	CA-CB-CG-CD

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	903	NAG	1	0
6	B	951[B]	ARG	1	0
5	A	902	NAG	1	0
5	B	906	NAG	1	1
5	B	902	NAG	1	0
5	A	901	NAG	1	0
6	D	951[A]	ARG	5	0
5	C	907	NAG	1	0
6	C	951	ARG	1	0
6	D	951[B]	ARG	1	0
6	B	951[A]	ARG	1	0
6	A	951	ARG	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, 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	421/461 (91%)	-0.23	0 100 100	23, 38, 60, 72	0
1	C	426/461 (92%)	-0.28	0 100 100	22, 35, 59, 77	1 (0%)
2	B	452/478 (94%)	0.15	5 (1%) 78 74	29, 53, 79, 94	0
2	D	441/478 (92%)	0.10	13 (2%) 53 48	23, 48, 91, 109	0
3	H	219/225 (97%)	-0.14	2 (0%) 81 78	21, 44, 69, 80	0
3	J	220/225 (97%)	-0.13	4 (1%) 67 63	23, 41, 66, 80	0
4	K	216/217 (99%)	-0.41	0 100 100	22, 34, 52, 66	0
4	L	216/217 (99%)	-0.24	0 100 100	18, 39, 65, 78	0
All	All	2611/2762 (94%)	-0.12	24 (0%) 81 78	18, 41, 73, 109	1 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	21	PRO	3.4
2	D	244	GLY	3.3
2	B	364	TRP	3.2
2	D	212	VAL	3.1
2	D	211	TRP	2.9

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
5	NAG	A	902	14/15	0.60	0.17	103,115,126,127	0
5	NAG	C	908	14/15	0.62	0.18	60,76,86,88	0
5	NAG	D	904	14/15	0.67	0.15	85,101,115,117	0
5	NAG	A	903	14/15	0.68	0.17	92,100,112,115	0
5	NAG	B	905	14/15	0.70	0.12	80,93,109,116	0
5	NAG	C	902	14/15	0.73	0.15	88,100,110,118	0
5	NAG	C	903	14/15	0.74	0.16	66,78,81,82	0
5	NAG	B	901	14/15	0.76	0.19	103,119,124,126	0
5	NAG	B	907	14/15	0.76	0.18	85,97,105,107	0
5	NAG	B	904	14/15	0.76	0.21	86,100,102,106	0
5	NAG	B	903	14/15	0.77	0.14	88,101,113,113	0
5	NAG	B	906	14/15	0.78	0.17	89,99,104,104	0
5	NAG	A	905	14/15	0.78	0.14	71,86,95,97	0
5	NAG	D	903	14/15	0.79	0.13	43,62,71,73	0
5	NAG	C	907	14/15	0.80	0.13	58,67,79,85	0
7	NA	C	962	1/1	0.81	0.13	54,54,54,54	0
5	NAG	C	905	14/15	0.83	0.16	52,63,72,75	0
5	NAG	A	907	14/15	0.85	0.14	72,85,97,99	0
5	NAG	C	904	14/15	0.85	0.11	45,53,63,66	0
5	NAG	B	902	14/15	0.86	0.11	38,52,61,64	0
5	NAG	A	904	14/15	0.86	0.10	50,62,75,78	0
7	NA	A	962	1/1	0.86	0.17	60,60,60,60	0
5	NAG	D	901	14/15	0.86	0.12	39,52,68,70	0
5	NAG	A	906	14/15	0.87	0.11	37,51,61,66	0
6	ARG	D	951[A]	12/12	0.88	0.24	29,59,81,88	8
7	NA	C	961	1/1	0.88	0.17	37,37,37,37	0
6	ARG	D	951[B]	12/12	0.88	0.24	29,64,82,88	8
5	NAG	D	902	14/15	0.91	0.08	33,48,53,55	0
5	NAG	C	906	14/15	0.91	0.09	34,41,52,61	0
6	ARG	B	951[B]	12/12	0.92	0.18	35,70,78,81	8
6	ARG	B	951[A]	12/12	0.92	0.18	35,71,78,81	8
6	ARG	C	951	12/12	0.93	0.09	22,28,33,34	0
5	NAG	C	901	14/15	0.94	0.08	19,28,36,39	0
5	NAG	A	901	14/15	0.95	0.08	17,33,43,50	0
7	NA	A	961	1/1	0.96	0.08	34,34,34,34	0
6	ARG	A	951	12/12	0.96	0.07	20,30,35,37	0
8	CL	B	971	1/1	0.96	0.10	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CL	D	971	1/1	0.96	0.17	66,66,66,66	0
7	NA	D	961	1/1	0.97	0.04	37,37,37,37	0
9	CA	K	301	1/1	0.97	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.