wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:01 PM GMT

PDB ID	:	4WJL
Title	:	Structure of human dipeptidyl peptidase 10 (DPPY): a modulator of neuronal Kv4 channels
Authors	:	Bezerra, G.A.; Dobrovetsky, E.; Seitova, A.; Fedosyuk, S.; Dhe-Paganon, S.; Gruber, K.
Deposited on	:	2014-09-30
Resolution	:	3.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

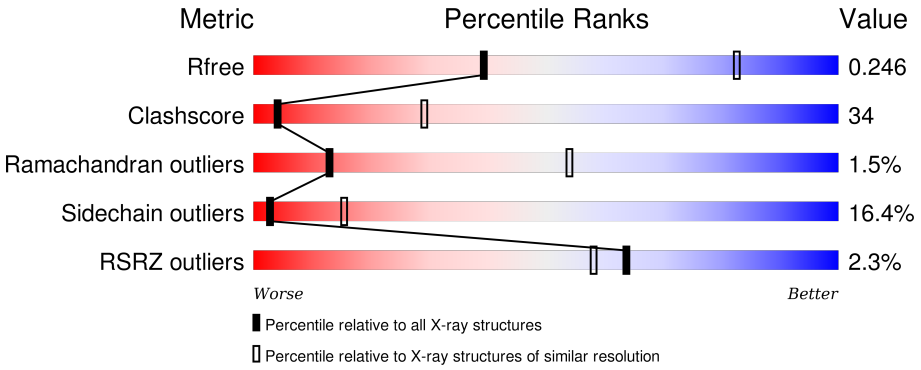
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 <=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	719	3% 45% 43% 11% •
1	B	719	2% 44% 45% 10% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11829 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.

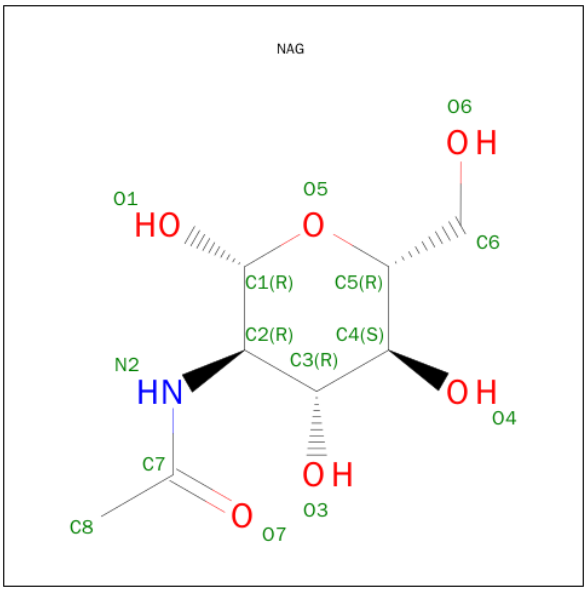
- Molecule 1 is a protein called Inactive dipeptidyl peptidase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	0	0	0
			5794	3730	959	1080	25			
1	B	719	Total	C	N	O	S	0	0	0
			5806	3736	960	1085	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	MET	VAL	variant	UNP Q8N608
A	401	ILE	VAL	variant	UNP Q8N608
B	288	MET	VAL	variant	UNP Q8N608
B	401	ILE	VAL	variant	UNP Q8N608

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total C N O 50 28 2 20	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total C N O 28 16 2 10	0	0
4	B	2	Total C N O 28 16 2 10	0	0
4	B	2	Total C N O 28 16 2 10	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

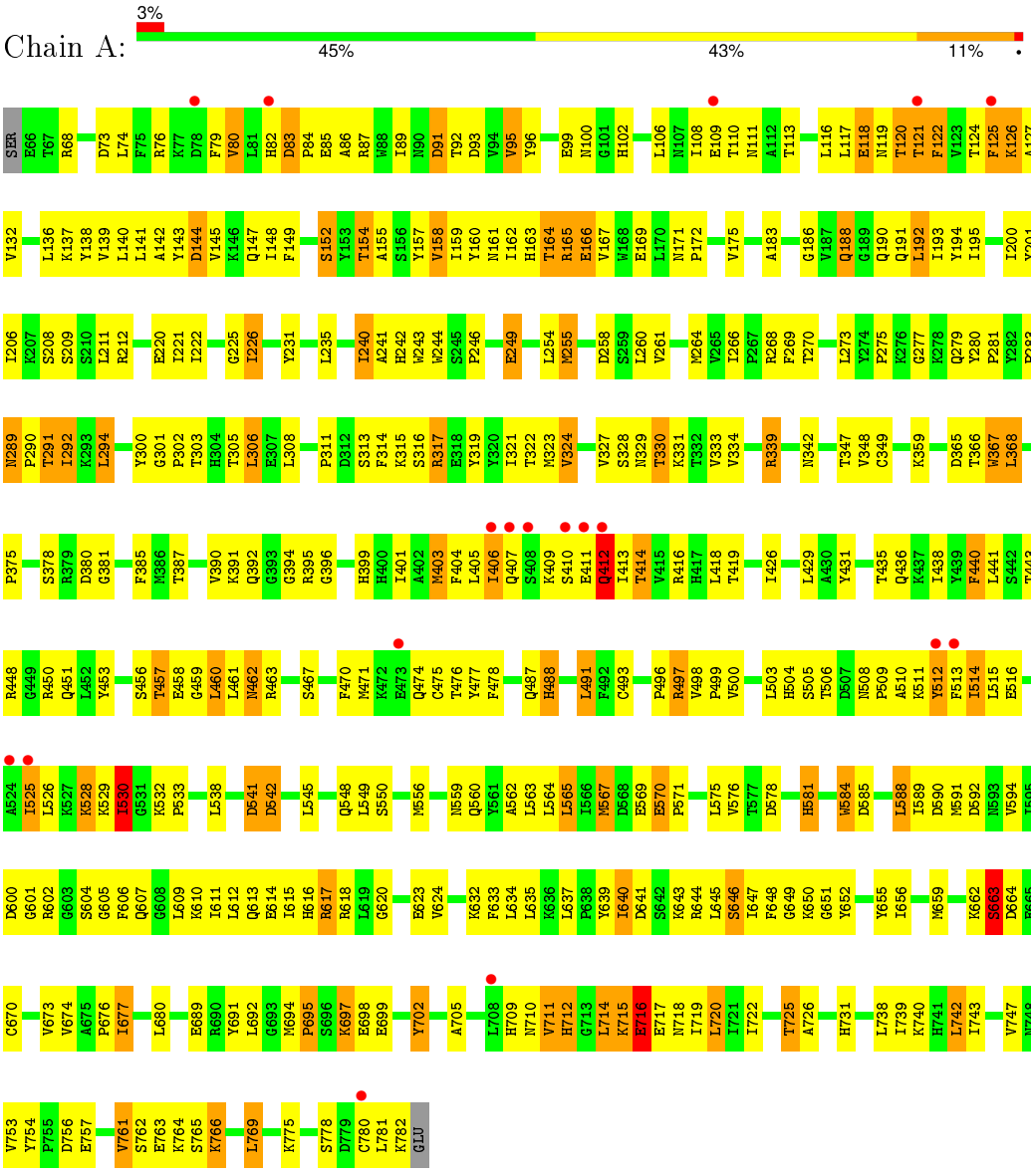
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total C N O 39 22 2 15	0	0

3 Residue-property plots (i)

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 (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.

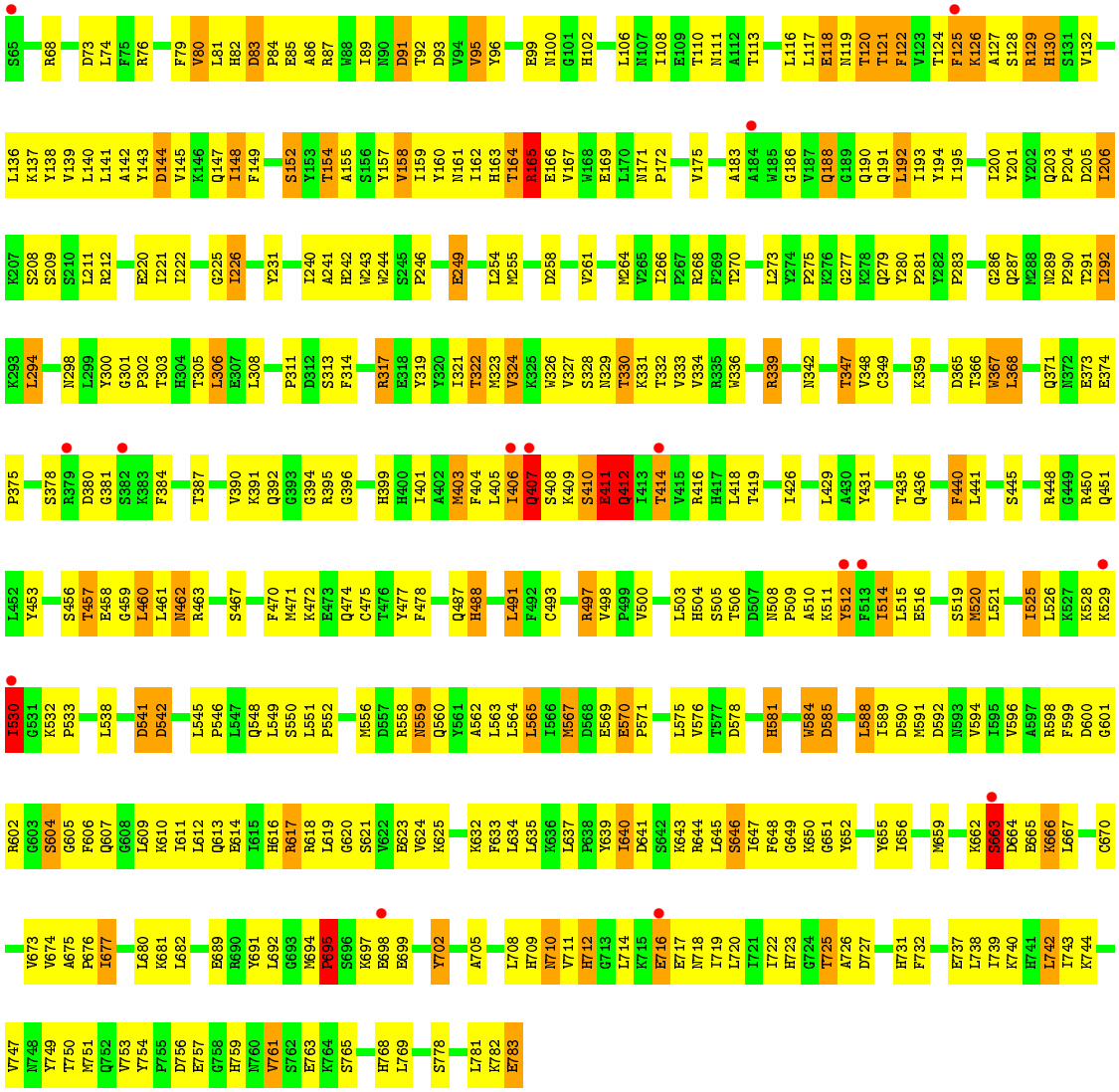
- Molecule 1: Inactive dipeptidyl peptidase 10

Chain A:



- Molecule 1: Inactive dipeptidyl peptidase 10

Chain B:


S65 R68 D73 L74 F75 R76 F79 V80 L81 H82 D83 P84 E85 A86 R87 W88 I89 N90 D91 T92 D93 V94 V95 Y96 E99 N100 G101 H102 L106 N107 I108 E109 T110 N111 A112 T113 L116 L117 E118 N119 T120 T121 F122 V123 T124 F125 K126 A127 S128 R129 H130 S131 V132
L136 K137 Y138 V139 L140 L141 A142 Y143 D144 V145 K146 Q147 I148 F149 S152 Y153 T154 A155 S156 Y157 V158 I159 Y160 N161 I162 H163 T164 R165 E166 V167 W168 E169 L170 N171 P172 V175 A183 A184 W185 G186 V187 Q188 G189 Q190 Q191 L192 I193 Y194 I195 I200 Y201 Y202 Q203 P204 D205 I206
K207 S208 S209 S210 L211 R212 E220 I221 I222 G225 I226 Y231 I240 A241 E242 W243 W244 S245 P246 E249 L254 M255 D258 V261 M264 V265 I266 P267 R268 F269 T270 L273 Y274 P275 K276 G277 K278 Q279 Y280 P281 Y282 P283 G286 Q287 M288 N289 P290 T291 I292
K293 L294 N298 L299 Y300 G301 P302 T303 H304 T305 L306 E307 L308 P311 D312 S313 F314 R317 E318 Y319 Y320 I321 T322 M323 V324 K325 W326 V327 S328 N329 T330 K331 T332 V333 V334 R335 W336 R339 N342 T347 C349 K359 D365 T366 W367 L368 Q371 N372 E373 E374
P375 S378 R379 D380 G381 S382 K383 F384 T387 V390 K391 Q392 G393 G394 R395 G396 H399 H400 I401 A402 M403 F404 L405 I406 Q407 S408 K409 S410 E411 Q412 I413 T414 V415 R416 H417 L418 T419 I426 L429 A430 Y431 T435 Q436 F440 L441 S445 R448 G449 R450 Q451
L452 Y453 S456 T457 E458 G459 L460 L461 N462 R463 S467 F470 M471 K472 E473 Q474 C475 T476 Y477 F478 Q487 H488 L491 F492 C493 R497 V498 P499 V500 L503 H504 S505 T506 D507 N508 P509 A510 K511 Y512 F513 I514 L515 E516 S519 M520 L521 I525 L526 K527 K528 K529
I530 G531 K532 P533 L538 D541 D542 L545 P546 L547 Q548 L549 S550 L551 P552 M556 D557 R558 N559 Q560 Y561 A562 L563 L564 L565 I566 M567 D568 E569 E570 P571 L575 V576 T577 D578 H581 W584 D585 L588 I589 D590 M591 D592 N593 V594 I595 V596 A597 R598 F599 D600 G601
R602 G603 S604 G605 F606 Q607 G608 L609 K610 I611 L612 Q613 E614 I615 H616 R617 R618 L619 G620 S621 V622 E623 V624 K625 K632 F633 L634 L635 K636 L637 P638 Y639 I640 D641 S642 K643 R644 L645 S646 I647 F648 G649 K650 G651 Y652 Y655 I656 M659 K662 S663 D664 E665 K666 L667 C670
V673 V674 A675 P676 I677 L680 K681 L682 E689 R690 Y691 L692 G693 M694 R695 S696 K697 E698 E699 Y702 A705 L708 H709 N710 V711 H712 G713 L714 K715 E716 E717 N718 I719 L720 I721 I722 H723 G724 T725 A726 D727 H731 F732 E737 L738 I739 K740 H741 L742 I743 K744
V747 N748 Y749 T750 M751 Q752 V753 Y754 F755 D756 E757 G758 H759 N760 V761 S762 E763 K764 S765 H768 L769 S778 L781 K782 E783

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.91Å 143.73Å 176.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.55 – 3.40 66.55 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.55-3.40) 99.9 (66.55-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.207 , 0.242 0.226 , 0.246	Depositor DCC
R_{free} test set	1476 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 28971 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11829	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.39	0/5940	0.63	1/8052 (0.0%)
1	B	0.41	0/5952	0.64	1/8069 (0.0%)
All	All	0.40	0/11892	0.63	2/16121 (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	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	585	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	714	LEU	N-CA-C	-5.20	96.95	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	GLN	Mainchain,Peptide
1	B	407	GLN	Peptide
1	B	412	GLN	Mainchain
1	B	695	PRO	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	710	ASN	Mainchain

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	5794	0	5719	404	0
1	B	5806	0	5720	392	0
2	A	28	0	26	1	0
2	B	28	0	26	6	0
3	A	50	0	43	4	0
4	A	28	0	25	4	0
4	B	56	0	50	7	0
5	B	39	0	34	4	0
All	All	11829	0	11643	794	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 34.

The worst 5 of 794 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:165:ARG:H	1:A:165:ARG:CD	1.60	1.14
1:A:165:ARG:H	1:A:165:ARG:HD2	1.08	1.08
1:A:488:HIS:HB3	1:A:505:SER:HA	1.38	1.05
1:A:644:ARG:HD2	1:A:781:LEU:O	1.57	1.04
1:B:488:HIS:HB3	1:B:505:SER:HA	1.39	1.03

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	715/719 (99%)	632 (88%)	71 (10%)	12 (2%)	11 51
1	B	717/719 (100%)	635 (89%)	72 (10%)	10 (1%)	14 55
All	All	1432/1438 (100%)	1267 (88%)	143 (10%)	22 (2%)	13 54

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	A	413	ILE
1	A	663	SER
1	A	711	VAL
1	B	165	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	645/650 (99%)	540 (84%)	105 (16%)	3 16
1	B	646/650 (99%)	539 (83%)	107 (17%)	3 15
All	All	1291/1300 (99%)	1079 (84%)	212 (16%)	3 15

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	711	VAL
1	B	128	SER
1	B	635	LEU
1	A	720	LEU
1	B	95	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	B	287	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

13 carbohydrates are modelled in this entry.

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	$\#\|Z\|>2$
3	NAG	A	803	1,3	14,14,15	0.47	0	15,19,21	1.72	2 (13%)
3	NAG	A	804	3	14,14,15	0.61	0	15,19,21	1.52	2 (13%)
3	BMA	A	805	3	11,11,12	0.67	0	14,15,17	2.83	5 (35%)
3	MAN	A	806	3	11,11,12	0.45	0	14,15,17	1.71	3 (21%)
4	NAG	A	807	1,4	14,14,15	0.60	0	15,19,21	0.97	1 (6%)
4	NAG	A	808	4	14,14,15	0.54	0	15,19,21	1.52	1 (6%)
4	NAG	B	802	1,4	14,14,15	0.75	1 (7%)	15,19,21	1.12	1 (6%)
4	NAG	B	803	4	14,14,15	0.53	0	15,19,21	0.76	0
5	NAG	B	804	1,5	14,14,15	0.71	0	15,19,21	0.98	1 (6%)
5	NAG	B	805	5	14,14,15	0.63	0	15,19,21	0.73	0
5	BMA	B	806	5	11,11,12	0.52	0	14,15,17	1.39	1 (7%)
4	NAG	B	807	1,4	14,14,15	0.62	0	15,19,21	1.56	4 (26%)
4	NAG	B	808	4	14,14,15	0.45	0	15,19,21	1.63	1 (6%)

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
3	NAG	A	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	804	3	-	0/6/23/26	0/1/1/1
3	BMA	A	805	3	-	0/2/19/22	0/1/1/1
3	MAN	A	806	3	-	0/2/19/22	1/1/1/1
4	NAG	A	807	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	808	4	-	2/6/23/26	0/1/1/1
4	NAG	B	802	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	803	4	-	0/6/23/26	0/1/1/1
5	NAG	B	804	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	805	5	-	0/6/23/26	0/1/1/1
5	BMA	B	806	5	-	0/2/19/22	0/1/1/1
4	NAG	B	807	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	808	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	NAG	C1-C2	2.07	1.55	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	805	BMA	C1-C2-C3	-8.47	99.52	109.54
3	A	803	NAG	C2-N2-C7	-5.89	115.47	123.04
4	B	807	NAG	C4-C3-C2	-2.50	107.34	111.23
5	B	804	NAG	C2-N2-C7	-2.26	120.14	123.04
3	A	806	MAN	C2-C3-C4	-2.21	107.29	111.04

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	808	NAG	C8-C7-N2-C2
4	B	802	NAG	C8-C7-N2-C2
4	B	802	NAG	O7-C7-N2-C2
4	A	808	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	806	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	NAG	2	0
3	A	804	NAG	2	0
3	A	805	BMA	1	0
3	A	806	MAN	1	0
4	A	807	NAG	4	0
4	A	808	NAG	4	0
4	B	802	NAG	3	0
5	B	804	NAG	3	0
5	B	805	NAG	3	0
5	B	806	BMA	1	0
4	B	807	NAG	4	0
4	B	808	NAG	4	0

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	NAG	A	801	1	14,14,15	0.62	0	15,19,21	0.90	0
2	NAG	A	802	1	14,14,15	0.55	0	15,19,21	1.46	3 (20%)
2	NAG	B	801	1	14,14,15	0.41	0	15,19,21	1.93	2 (13%)
2	NAG	B	809	1	14,14,15	0.59	0	15,19,21	1.50	3 (20%)

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
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	2/6/23/26	0/1/1/1
2	NAG	B	809	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	809	NAG	C6-C5-C4	-3.36	104.74	113.02
2	A	802	NAG	C3-C2-N2	2.22	115.89	110.56
2	B	801	NAG	C2-N2-C7	2.27	125.95	123.04
2	A	802	NAG	O5-C5-C6	2.30	112.33	107.35
2	B	809	NAG	C3-C4-C5	2.45	114.47	110.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	NAG	C8-C7-N2-C2
2	B	801	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	1	0
2	B	809	NAG	6	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^{th} 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	717/719 (99%)	0.24	18 (2%)	61	55	33, 69, 138, 251	19 (2%)
1	B	719/719 (100%)	0.28	15 (2%)	67	61	32, 67, 129, 227	11 (1%)
All	All	1436/1438 (99%)	0.26	33 (2%)	64	58	32, 68, 131, 251	30 (2%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	GLN	6.3
1	A	411	GLU	4.9
1	B	716	GLU	4.8
1	B	65	SER	4.6
1	A	408	SER	4.5

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	B	807	14/15	0.93	0.22	0.68	71,71,71,71	0
5	NAG	B	804	14/15	0.87	0.26	-0.03	83,83,83,83	0
4	NAG	A	807	14/15	0.92	0.21	-0.41	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	803	14/15	0.92	0.15	-1.90	74,74,74,74	0
3	MAN	A	806	11/12	0.72	0.28	-	113,113,113,113	0
4	NAG	B	803	14/15	0.80	0.34	-	128,128,128,128	0
3	BMA	A	805	11/12	0.83	0.22	-	135,135,135,135	0
5	NAG	B	805	14/15	0.87	0.31	-	113,113,113,113	0
5	BMA	B	806	11/12	0.81	0.24	-	127,127,127,127	0
4	NAG	B	802	14/15	0.93	0.19	-	69,69,69,69	0
4	NAG	A	808	14/15	0.73	0.27	-	131,131,131,131	0
4	NAG	B	808	14/15	0.84	0.26	-	128,128,128,128	0
3	NAG	A	804	14/15	0.88	0.20	-	88,88,88,88	0

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	801	14/15	0.83	0.27	-	109,109,109,109	0
2	NAG	A	802	14/15	0.89	0.26	-	84,84,84,84	0
2	NAG	B	809	14/15	0.73	0.48	-	189,189,189,189	0
2	NAG	B	801	14/15	0.84	0.25	-	106,106,106,106	0

6.5 Other polymers (i)

There are no such residues in this entry.